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CPM User's Guide

[PDF of User's Guide.](#)

Welcome to the EPA's Superfund "Counts Per Minute (CPM) Calculator" user's guide. Here you will find instructions on how to use the calculator and supporting technical documentation explaining the conversion to cpm process. Additional guidance is also provided on the limitations and intended use of this calculator. It is suggested that users read the [CPM FAQ](#) page before proceeding. The user guide is extensive so please use the "Open All Sections" and "Close All Sections" links below as needed. Individual sections can be opened and closed by clicking on the section titles. Before proceeding through the user's guide please read the [Disclaimer](#).

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Disclaimer

This guidance document sets forth EPA's recommended approaches based upon currently available information with respect to estimating detector readings that correspond to remedial criteria at Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) sites (commonly known as Superfund). This document does not establish binding rules. Alternative approaches for estimating detector readings may be found to be more appropriate at specific sites (e.g., where site circumstances do not match the underlying assumptions, conditions and models of this guidance). The decision whether to use an alternative approach and a description of any such approach should be documented. Accordingly, when comments are received at individual sites questioning the use of the approaches recommended in this guidance, the comments should be considered and an explanation provided for the selected approach.

The policies set out in the CPM User's Guide provide guidance to EPA staff. It also provides guidance to the public and regulated community on how EPA intends estimating detector readings to be implemented. EPA may change this guidance in the future, as appropriate.

It should also be noted that estimating detector readings is not intended to replace sampling. Verification samples are still required. The CPM Calculator has many limitations that are detailed in the user's guide. Use of the CPM output is intended to reduce the number of laboratory samples and not eliminate them.

This web calculator may be used to estimate detector readings for radionuclides in several different media. The calculator is flexible and may be used to derive site-specific detector readings as more site characterization is obtained. This is particularly true where the contamination source depth from surface varies.

1. Introduction

Field sampling is a necessary step of environmental remediation. Field sampling establishes areas of contamination before, during, and after site characterization in order to ensure only acceptable residual levels of contamination remain. Sampling has the potential to be an extremely time-consuming and expensive portion of a radiological site remediation. Collected samples must be shipped to an off-site laboratory or counted in an on-site mobile unit in order to establish areas of contamination and to ensure that remaining contaminants are of acceptable residual levels. This tool is provided to help calculate the radiation detector reading in counts per minute (cpm) that corresponds to the level of radioactivity in a surface or volume of medium by converting radioactivity in either pCi/cm² or pCi/g to cpm.

The CPM Calculator is a web-based calculator that estimates a gamma detector response for a target level of contamination in a source medium. This calculator can be used to determine screening levels in cpm that are based on pCi per volume or area. Using handheld detectors measuring cpm can help reduce costly laboratory sampling. A correction factor for cpm analysis established between this calculator's results and lab sampling analysis may be needed to account for ground truthing and other field nuances like roughness factors.

The user should always verify CPM Calculator results with lab sampling.

Features of the CPM Calculator include:

- option to calculate the Gross Detector Response (GDR) for a single radionuclide or multiple radionuclide mixtures according to MARSSIM guidance,
- option to include daughter ingrowth,
- choice of target activity,
- truncated decay chains, which allow for man-made decay spectrum,
- inclusion of 3 natural decay series (U-235, U-238, and Th-232),

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- choice between 4 gamma NaI crystal detector sizes (0.5x1, 1x1, 2x2, 3x3 inch),
- choice of 7 contamination depths (ground plane, 1, 2, 3, 5, 15, infinite depth),
- choice of 6 source materials (soil, steel, concrete, glass, wood, drywall), and
- exact data for 11 radionuclides most commonly found at remediation sites.

2. Understanding the CPM Calculator

This section presents a general overview of the CPM Calculator. See section 4 for greater detail.

2.1 General Considerations

The gross detector response (GDR) is produced by the CPM calculator for the isotopes and activity concentrations selected to represent the site. The GDR is calculated from MCNP simulations that derive a conversion factor (FC) representative of the media, detector size, distance from the source, and depth of source contamination from the surface. With multiple variables, limitations of the tool are expected.

2.2 Limitations of the CPM Calculator

Limitations of the GDR calculations are discussed here. It is expected that a correction factor be derived based on differences between the theoretical GDR value from the CPM Calculator and the site measured CPM.

2.2.1 The Model

The Volume CPM Calculator model was developed using 248 case runs of MCNP to simulate the spectrum of the desired radionuclide(s). The Volume CPM Calculator does not replace the need for lab-based sampling or MARSSIM final status survey requirements; however, it may provide a reasonable starting point from which to work. A correction factor for cpm analysis established between this calculator's results and lab sampling analysis should be applied to account for this simulation as well as ground truthing and other field nuances.

2.2.2 Uniformity

The model assumes uniform contamination on the source surface. In other words, the radionuclides of interest are in constant ratio to each other on the surface and the source surface is infinite in lateral extent. Incongruity of the radionuclide ratios, such as separate spills or cross-contaminated sites, will diminish the effectiveness of the calculator.

2.2.3 Gamma Emitters

Radionuclides that emit alpha and beta radiation are difficult to measure with any accuracy in the field and are omitted from this model unless the radionuclide also emits a qualifying gamma particle.

A qualifying gamma particle is one with energy between 20 keV and 3 MeV and with a decay yield greater than 0.1%. The energy cutoff is due to the energy response curve given in the model detector manufacturer's specifications. For more information, see the FAQs.

Bremsstrahlung radiation is electromagnetic radiation produced by the deceleration of a charged particle when deflected by another charged particle, typically an electron deflected by an atomic nucleus. The moving particle loses kinetic energy and is then converted into a photon. A study of the contribution of this radiation from the modeled materials is in progress.

2.2.4 Background Radiation

The model does not account for background radiation. The user is responsible for adding or subtracting any background counts to the GDR.

2.3 CPM Output

See section 3 for detailed information on running the calculator and interpreting the output.

2.4 Radionuclide-Specific Parameters

Several radionuclide-specific parameters are needed for development of the GDRs. The parameters sources are identified here.

1. Half-life (yr), Decay mode, Atomic weight, Atomic number and Decay energy. [ICRP 107](#).
2. Photon energy and yield. The values used are available [here](#). The first column presents the photon energy in MeV. The second column presents the photon yield in %/nt. [ICRP 107](#)

2.5 CPM results in the Context of Superfund Modeling Framework

This CPM calculator focuses on the estimation of detector readings that may be used as part of the larger framework determining if a site complies with remediation criteria. Criteria that can be converted to cpm in this tool can come from

the PRG, BPRG, SPRG, DCC, BDCC, and SDCC Calculators or concentrations in ARARs. The user's guides for these calculators should be consulted prior to entering their results as Target Activity Concentrations in the CPM Calculator.

Prior to using another model for GDR at a CERCLA remedial site, EPA regional staff, should consult with the Superfund remedial program's National Radiation Expert (Stuart Walker, at (703) 603-8748 or walker.stuart@epa.gov).

3. Using the CPM Website

This section provides the user with a step by step guide for each page of the CPM calculator and highlights potential issues that may be encountered.

3.1 Selecting Radionuclides of Interest

There are two picklists to choose from. The first one includes all isotopes that are available. The second one includes common radionuclides found at Superfund sites. To select a radionuclide, click on it's name to highlight the selection. Next, click the blue bottom with arrows to move that radionuclide to the RAdionuclide of Interest box. Multiple radionuclides can be moved together by holding the shift or control keys while clicking on radionuclide names. To remove a radionuclide from the radionuclides of interest box, highlight it and click the blue button with the arrows pointing back to the picklist.

Place a checkmark in the "Include daughter products" box if it is suspected that progeny will be present. Selecting this option will include all the progeny at their fractional relationship to the parent. Daughter products that reach secular equilibrium in a hundred to a thousand years are automatically added. Adding a parent and its daughter will automatically deselect the daughter, as it is inherently included. To calculate the parent and daughter activities manually, deselect the box "Include daughter products." Chains with very long-lived daughters have been truncated at the typical 'parent' radionuclides for man-made purposes. To select one of three natural decay series, find the parent with the suffix of 'nat'.

The following 11 radionuclides are the most common photon emitting nuclides found at Superfund remedial sites: Am-241, Cs-137, I-131, Ra-226, Ra-228, Rn-220, Th-230, Th-232, U-234, U-235, and U-238. These radionuclides were modeled with their exact photon spectrum, which is used rather than simulating the photon spectrum as is done with the other radionuclides.

Before leaving the page you will be asked to check the box that asks you if you have read the user's guide and FAQ to grasp the limitations and intended use of the calculator.

When all the desired radionuclides have been selected, click "Next".

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☒ I have read and understand the limitations of this model set forth in the User Guide and FAQ.

Radionuclides
(and daughter progeny)

Ac-223
Ac-224
Ac-225
Ac-226
Ac-227
Ac-228
Ag-102
Ag-103
Ag-104
Ag-104m

<<>>

Radionuclides of Interest

Am-241
U-238

<<>>

Common
Radionuclides

Co-60
Cs-137
Pu-238
Pu-239
Pu-240
Ra-226
Ra-228
Rn-220
Rn-222
Tc-99

<<>>

☒ Include daughter products (Recommended)

m = metastable state
n = second metastable state

Next

3.2 Target and Field Activity Concentrations

Enter the target activity concentrations (TAC) in pCi/cm² or pCi/g for each radionuclide. The TAC is the activity for which the result in cpm is desired. The TAC may be concentrations developed using the following EPA Calculators or concentrations specified in an ARAR.

- the [PRG](#) Calculator for radionuclide cancer risk for soil,
- the [DCC](#) Calculator should be used to assess radionuclide dose for soil,
- the [BPRG](#) Calculator for radionuclide cancer risk inside buildings,
- the [BDCC](#) Calculator for radionuclide dose inside buildings,
- the [SPRG](#) Calculator should be used to assess radionuclide cancer risk for hard outside surfaces, and
- the [SDCC](#) Calculator for radionuclide dose for hard outside surfaces.

If multiple radionuclides are selected, enter the field activity concentration (FAC) for each radionuclide. The FAC is based on laboratory analysis. The FAC is the activity of each primary radionuclide in the contaminated source and is used to find the radionuclide ratios in mixtures. The FACs are used to find the relative fractions of each radionuclide, which are then applied to the GDR. Click "Next".

https://epa-cpm.ornl.gov:8085/users_guide.html[8/11/2022 1:11:05 PM]

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Radionuclide	Field Activity Concentration	Target Activity Concentration
Am-241	<input type="text" value="45"/>	<input type="text" value="25"/>
U-238	<input type="text" value="25"/>	<input type="text" value="5"/>

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3.3 Detector and Material Information

On this page the details of the detector used and the details of contaminated media are required.

- Select the source material of interest
- Select the uniform depth of contamination in the source material
- Select the gamma scintillation detector size
- Select the detector height above the source.
- Click "Next".

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Detector Specifications	
Select Source Material	<div>Soil</div>
Select Source Depth	<div>Infinite</div>
Select Detector size	<div>2 x 2</div>
Select Detector Height	<div>1 cm</div>

Soil

Steel

Concrete

Glass

Wood

Drywall

1 cm

2 cm

3 cm

5 cm

15 cm

Ground Plane

Infinite

0.5 x 1

1 x 1

2 x 2

3 x 3

0.5 cm

1 cm

2.54 cm

10 cm

30 cm

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3.4 Results - Gross Detector Response

On this page the GDR is given that approximates meeting the TAC for the radionuclides selected. The inputs for source material, source depth, detector size, and detector height are repeated. Additionally, the photon energy and yield are presented if one clicks on the highlighted numbers. If any photon energies are out of the range of the detector, they are identified.

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Input and calculation parameters								
Radiouclide	Daughter	Fractional Activity of Parent	Number of Photons	CF (CPM/pCi)	Field Activity (pCi/g)	Target Activity (pCi/g)	Field Activity (CPM)	Target Activity (CPM)
Am-241			1	1.008e+2	25	25	4535	2519
U-238			0	2.240e-1	5	5	6	1
	Th-234	1.000E+00	4	5.669e+1				
	Pa-234m	9.974E-01	4	4.576e+1				
	Pa-234	4.157E-03	53	4.812e+3				

Gross Detector Response for user supplied detector parameters	
Source Material	Soil
Source Depth	Infinite
Detector Size	2 x 2 in
Detector Height	1 cm
Gross Detector Response (CPM)	582

- Gross Detector Response (GDR) is the instrument reading that must be achieved in order to meet the target activity entered by the user.

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Start Over

4. Technical Documentation

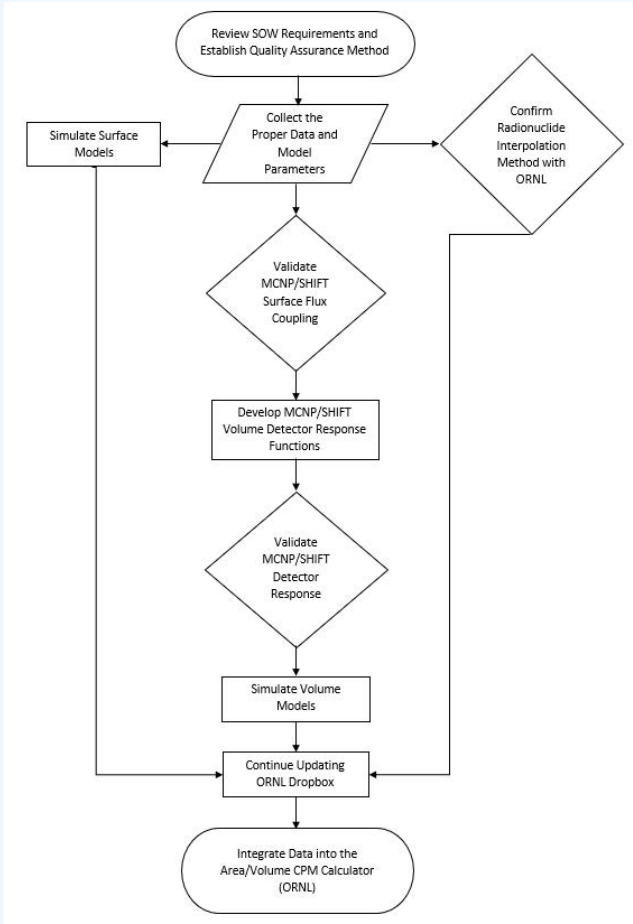
This section presents the details of the GDR calculation process and validation of the method.

4.1 Overview of Design

The goal of the validation effort is to simulate a detector count rate that would be normalized to an activity concentration on the surface area or in a volumetric depth of the media of interest for use in the CPM Calculator. The MCNP v6.2 radiation transport code has been utilized for validation modeling of the CPM surface calculator by simulating the energy deposition (F8) pulse height tally (Werner et al., 2017). A benchmark of Shift capabilities indicated that radiation transport of photons through contaminated volumetric depths, as required in the Volume CPM function, supersedes capabilities of MCNP by at speed factor of 10 for simulations of track length estimate of cell flux. The ability to conduct rapid, high-fidelity radiation transport simulations is paramount for this initiative given the desired 23,120 discrete simulations for a series of contamination depths, 19 monoenergetic photon energies, 17 gamma-ray emitting radionuclides, and four NaI(Tl) detector models.

Only primary gamma-ray emissions were considered due to Shift's capability to conduct neutral particle, and not charged particle transport. Since Shift currently does not support a pulse height tally, a detector response function to generate detector count rates was developed. Any primary or secondary charged particle transport requires the use of MC code (e.g. MCNP). Therefore, beta emissions from the list of radionuclides, as well as pure beta-emitters (H-3 and

Sr-90) and their associated bremsstrahlung emissions cannot be run using Shift and were therefore not addressed in the simulations. In order to eliminate the computational runtime of simulating the gamma-ray emitting radionuclides in MCNP, an interpolation method was employed. In addition, both Rn-220 and Rn-222 lack the criteria described for photon emission and have also been eliminated. These criteria reduce the list of Superfund radionuclides of interest to the gamma-ray emitting radionuclides. A flow chart is provided below to summarize the methodology approach.



Parametric bounds for modeling were developed using the radiation transport codes Monte Carlo N-Particle (MCNP) and/or SHIFT for CPM calculator validation. SHIFT is the preferred transport code for validation modeling of the CPM Calculator. Parameters to be modeled include; plane radii, photon energies, discrete Superfund nuclides of interest (Am-241, Co-60, Ba-137m/Cs-137, Pu-238, Pu-239, Pu-240, Ra-226, Ra-228, Tc-99, Th-228, Th-230, Th-232, U-234, U-235, U-238/Pa-234m), and source material compositions. SHIFT modeling was performed for four NaI detectors (0.5x1, 1x1, 2x2, and 3x3-inch). Source-detector distances of 0.5 cm, 1 cm, 2.54 cm, 10 cm, 30 cm were modeled. Media of soil, concrete, wood, steel, drywall, and glass were evaluated for depths (source thicknesses) of ground plane, 1cm, 2cm, 3cm, 5cm, 15cm, and infinite. Nineteen discrete energies between 20 keV and 3 MeV were evaluated (0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.1, 0.15, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1.0, 1.5, 2.0, and 3.0 MeV). Photon energies were extrapolated for the values in between the discrete energies. The energies of the radionuclides selected by the user were applied to the detector response curves. The GDR was then calculated to meet the TAC. Details of the steps of this process are presented in the following sections.

The table below presents the source thicknesses that were considered for each media. For some material and energy combinations, the mass attenuation coefficient, and hence the infinite thickness, may exceed the the thickness considered. In the cases where the simulation thickness is less than four mean free paths, the media/source depth was not evaluated. Over the four detector sizes evaluated, 156 of the 23,120 possible combinations were not evaluated.

Material	Ground Plane	1cm	2cm	3cm	5cm	15cm	Infinite
Soil	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Concrete	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Wood	Yes	Yes	Yes	Yes	Yes	No	No
Steel	Yes	Yes	Yes	Yes	Yes	Yes	No
Glass	Yes	Yes	Yes	Yes	No	No	No
Drywall	Yes	Yes	Yes	Yes	No	No	No

Material	Monoenergetic Energies	Rdionuclide Energies	Contamination Depths	Detector Distances	Number of Detectors	Total Runs
Concrete	19	17	7	5	4	5,320
Drywall	19	17	4	5	4	3,040
Glass	19	17	4	5	4	3,040
Soil	19	17	7	5	4	5,320
Steel	19	17	7	5	4	5,320
Wood	19	17	5	5	4	3,800
Total						23,120

4.2 Design Testing and Benchmarking

Both MCNP and SHIFT software packages were considered for the CPM Calculator design. Each was tested and benchmarked against each other for repeatability and speed.

MCNP is a stochastic method that is widely used to solve radiation transport problems in reactor physics, shielding, dosimetry, radiation detection and measurements, and various other applications of interest. The Monte Carlo (MC) method enables detailed, explicit geometric, energy, and angular representations and hence is considered the most accurate method available for solving complex radiation transport problems (Wagner et al., 2011). MCNP functions by simulating the individual average particle behavior in a given environment based on sampling of the probability density of particles in phase space. The "behavior" of a particle may be described by the types of interactions (neutron capture, photon scatter, photon leakage, etc.) or "events" that are sampled from probability distributions containing transport data based on the selection of a pseudorandom number. In MCNP, the lifetime of an individual particle from birth until termination (due to absorption, escape from the problem boundary) is described as its random "history."

At the end of the simulation, the final average quantities of interest known as tallies (such as flux, detector pulse, dose, etc.) are estimated from the distribution of all histories and have an associated uncertainty (relative error) that is proportional to one over the square root of the total number of histories for statistically well-behaved simulations. Therefore, the uncertainty may be decreased by increasing the number of histories simulated in the problem to coincide with the "law of large numbers," where the sample mean approaches the population mean as the sample size increases. While MCNP is considered to be the most accurate method available for solving complex radiation transport problems, it possesses the inherent disadvantage of being computationally expensive as the required number of histories to reach proper convergence (less than 5% for detector pulse height) is increased for complex problems (X-5 Monte Carlo Team, 2003).

SHIFT is a massively parallel Monte Carlo radiation transport package that implements hybrid methods (deterministic coupled with stochastic) to obtain a faster and more accurate solution to problems of interest, as opposed to purely stochastic Monte Carlo. The hybrid methodology utilized in this study is known as the CADIS (Consistent Adjoint Driven Importance Sampling) method, which is a tally optimization method that relies on the discrete ordinates deterministic solver, Denovo, as part of the Exnihilo code suite to generate an adjoint flux and associated importance map for particles simulated in a given environment. Once the adjoint flux and importance map is generated, particles are more likely to be born in regions of higher importance in the simulation environment. The CADIS method is known to be 10-100,000 times more efficient than analog (no variance reduction) Monte Carlo based on tally figure of merit (FOM) comparisons (Biondo et al., 2017). The hybrid capabilities of SHIFT are particularly useful for speeding up the transport of sources that undergo significant attenuation in large problem geometries, as well as lowering the variance of tally results when compared to analog Monte Carlo. SHIFT is currently capable of neutral particle transport for only photons and neutrons and may be used to simulate select tallies that mirror those included in MCNP, such as average flux in a volumetric cell (F4 in MCNP).

A benchmark of SHIFT capabilities indicated that radiation transport of photons through contaminated volumetric depths, as required in the Volume CPM function, supersedes capabilities of MCNP by at speed factor of 10 for simulations of track length estimate of cell flux. The ability to conduct rapid, high-fidelity radiation transport simulations is paramount for this initiative given that the SOW request (revised per criteria for gamma-emitters) for 23,120 discrete simulations for a series of contamination depths, 19 monoenergetic photon energies, 17 gammaray emitting radionuclides, and four NaI(Tl) detector models, summarized Table 3. Gamma-ray emitters were alone considered from the list due to SHIFT's capability to conduct neutral particle, and not charged particle, transport. Any primary or secondary charged particle transport requires the use of Monte Carlo code (e.g. MCNP). Therefore, beta emissions from the list of radionuclides, as well as pure beta-emitters (H-3 and Sr-90) and their associated radiative components cannot be run using SHIFT. In addition, both Rn-220 and Rn-222 lack the criteria for photon emission and have also been eliminated as gamma-ray emitters. These criteria reduce the list of Superfund RADIONUCLIDES of interest to the gamma-ray emitting radionuclides.

Note that Bremsstrahlung beta (+/-) particle transport and annihilations from positron emissions, for the listed radionuclides, were not considered. Should photons from these actions be expected, further analysis would be necessary to accurately predict the GDR..

4.2.1 Denovo Deterministic Solver Overview

A 3-D discrete ordinates transport solver utilized in Shift, known as Denovo, discretizes (conversion of continuous space to equivalent discrete space) the steady-state Boltzmann transport equation in space, angle, and energy to approximate the adjoint fluxes (importance functions that describe the expected tally contribution of particles) that are used to generate variance reduction parameters for accelerating fixed-source MC simulations (Wagner et al., 2011). The CPM Calculator photon sources are fixed, following the matrix equation, i.e.,



as opposed to a k-eigenvalue sources, following the characteristic equation, i.e.,



For brevity, all equations shown to demonstrate Shift's capabilities are derived. The steady-state Boltzmann transport equation solved in Denovo is given by (Evans et al., 2010):



Here, the state is defined by the angular flux ψ , and the independent variables are $r = (x,y,z)$ (in centimeters); $\Omega = (\theta,\varphi)$ (in steradians); and E (in mega-electron-volts) representing space, angle, and energy, respectively (Evans et al., 2010). This equation may be used to describe how various particle types (i.e., neutrons, photons) travel through a medium. The left-hand side terms of the above equation describe the net transport (leakage) and total interactions that the particle undergoes, respectively. The right-hand side of the above equation describes the total accumulated source density. The above equation is converted to a discrete angular form that accounts for anisotropic scattering of the source within a problem geometry as shown (Evans et al., 2010):



In simple terms, the above equation represents the continuous steady-state Boltzmann transport equation in a discrete space, such that Denovo can solve for the flux component through discretization over the problem geometry "mesh" that is defined by the user with respect to space and angle. The left- and right-hand sides of the above equation follow the same principle described by the above equation, where left-hand side describes the net transport (leakage) and total interactions that the particle undergoes, and the right-hand side describes the total accumulated source density. The equation above accounts for group (g) scattering (with respect to energy and angle), as well as even and odd spherical harmonics functions (Y^e, Y^o) used to evaluate Legendre polynomials that expand the angular flux scattering cross section.

The above equation may be expressed in operator form (Evans et al., 2010):



The same principle applies, where "L" represents the differential transport operator describing the net transport and total interactions of the source (left-hand side of the above equations). The "M" operator is used to convert the harmonic moments to discrete angles; the "S" operator defines the group transfer cross sections for particles (scattering from one energy group to another), and q_e represents the external source term (for photons this is negligible in the current study). The above equation may be further expanded to depict what Denovo is solving in matrix form (Evans et al., 2010):



The goal is to solve for the angular flux groups, given by $[\psi]_G$. Shift couples SCALE continuous-energy (Shift MC solver) and multigroup physics (Shift MC solver and Denovo deterministic solver) cross section libraries for hybrid transport. The CPM Calculator photon sources discretized in Denovo are separable energy-space isotropic sources, which facilitate the hybrid methods. As opposed to traditional (S_n) iterative discretization methods, Denovo utilizes the Koch-Baker-Alcouffe (KBA) parallel sweep algorithm to perform a 2-D decomposition of a 3-D cartesian orthogonal structured spatial mesh (i.e., the simulation problem space) to solve the steady-state Boltzmann transport equation in space, angle, and energy (Evans et al., 2010). In other words, the KBA algorithm directly inverts the "L" term in Eq. 6 to obtain a more computationally efficient solution of the angular flux by "sweeping" through the 3-D cartesian orthogonal structured spatial mesh, as opposed to traditional source iteration techniques that may take longer converge. The defined 3-D mesh in Shift is decomposed into computational domain blocks defined by the user that scale with the number of processors, as shown below (Evans et al., 2010):



The I, J, and K terms represent the total, global number of cells in the x-, y-, and z-direction respectively. The I_b, J_b , and K_b terms represent the size of each x-, y-, and z-domain on each processor, which are defined by the user. The number of "small blocks" previously mentioned that discrete ordinates methods visualize in the phase space to transport particles, denoted by I, J, and K are automatically calculated. The KBA decomposition may be visually depicted by the following figure.

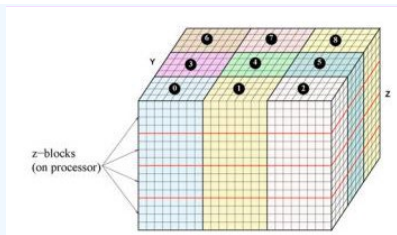


Figure 2. Decomposition of 3-D mesh for KBA. In this example, the grid is decomposed on nine processors.

The red lines (thick gray lines) indicate computational blocks in the z direction. Each processor has $I_b \times J_b \times K_b$ cells, and each block has size $I_b \times J_b \times K_b$ (Evans et al., 2010).

It should be noted that great care should be taken when defining the Denovo spatial mesh; a coarse mesh may result in unreliable importance maps even when source biasing is implemented. The Denovo deterministic solver also utilizes a ray tracing method to generate track-length contributions (i.e., mean free path determinations) within the geometry of the problem; increasing the number of rays fired per computational domain block (mesh face) is particularly useful for large problems with small tally volumes. This is especially prevalent with the 0.5x1 and 1x1-inch detector CPM Calculator simulations.

4.2.2 CADIS Hybrid Method Overview

The hybrid capabilities of Shift are particularly useful for speeding up the transport of sources that undergo significant attenuation in large problem geometries, as well as lowering the uncertainty associated with tally results when compared to analog (no variance reduction) MC. Shift is currently capable of neutral particle transport for only photons and neutrons and may be used to simulate select tallies that mirror those included in MCNP, such as average flux in a volumetric cell (F4 tally in MCNP). The hybrid methodology utilized in this study is known as the CADIS (Consistent Adjoint Driven Importance Sampling) hybrid method, which is a single tally region optimization method that relies on the discrete ordinates deterministic solver, Denovo, to generate an adjoint flux and associated importance map for particles simulated in a given environment. Once the adjoint flux and importance map are generated, particles are more likely to be born in regions of higher importance in the simulation environment. Omnibus code is used to couple the Denovo deterministic and Shift MC solver as part of the Exnihilo code suite to accelerate the Shift transport simulations. The CADIS hybrid method is known to be nearly 100,000 times more efficient than analog MC based on tally figure of merit (FOM) comparisons (Wagner et al., 2011).

In the CADIS method, particles are biased (increasing the number of sampled particles in order to decrease uncertainty). The biased source distribution is utilized such that particles are more likely to contribute to the total detector response and fall within the initial statistical weights (quantifies the tally contribution of particles in a simulation environment) generated from Denovo. The biased source distribution relationship is represented by the equations below (Wagner et al., 2011):



In the CADIS hybrid method, a weight window technique is applied by generating detailed space- and energy-dependent importance parameters (particle weights) and applying geometric splitting/roulette and energy splitting/roulette, while simultaneously controlling weight variations as a particle travels throughout an environment (Wagner et al., 2011). The deterministic Denovo solver generates the adjoint flux and associated weight window map; the Shift MC solver employs the stochastic splitting/roulette method in the phase space to determine the final contribution of particles in a tally region. The initial statistical weight of a particle is, $w_0(r \rightarrow, E)$, is defined by the following equation (Wagner et al., 2011):



Upon initiation of the Shift MC solver, if a particle falls below a given weight in the importance map (3-D distribution of $w_0(r \rightarrow, E)$), then the particle will be split (source biasing) or rouletted (terminated) in order to sufficiently increase its weight. This hybrid technique greatly increases the rate at which the Shift MC solver final solution converges, and thus significantly increases computational efficiency.

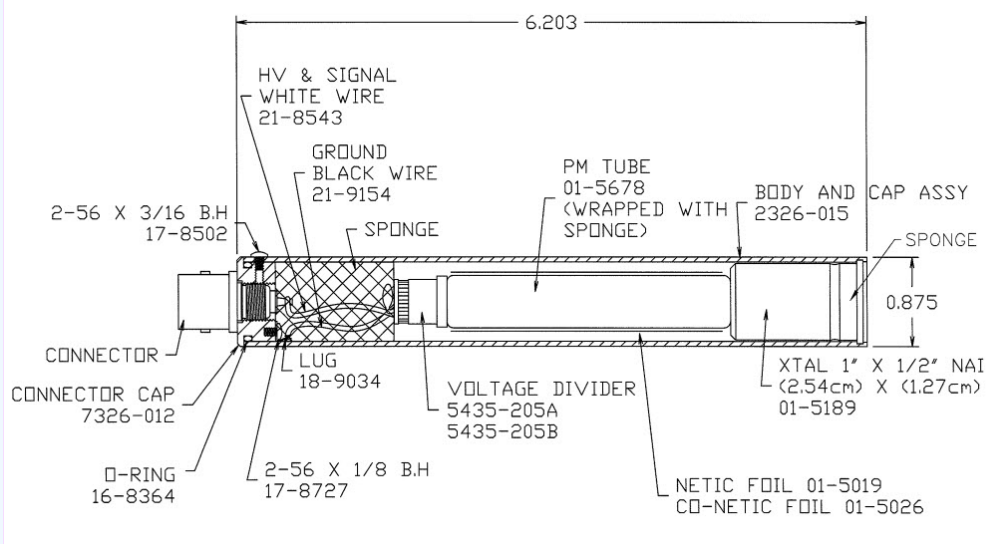
4.3 Detector Details

Four sodium iodine (NaI) detector sizes are included in the CPM Calculator (0.5x1-, 1x1-, 2x2-, and 3x3-inch). A detector response model for the 19 monoenergetic photons was created for each one using a pulse height energy deposition tally in MCNP. Once a representative detector was developed, a reliable relationship between the MCNP F8 pulse height tally and average cell flux to convert to a Shift average cell flux was established. Click the model number to see the response curves.

- Ludlum model [44-62](#) 0.5x1 inch NaI detector



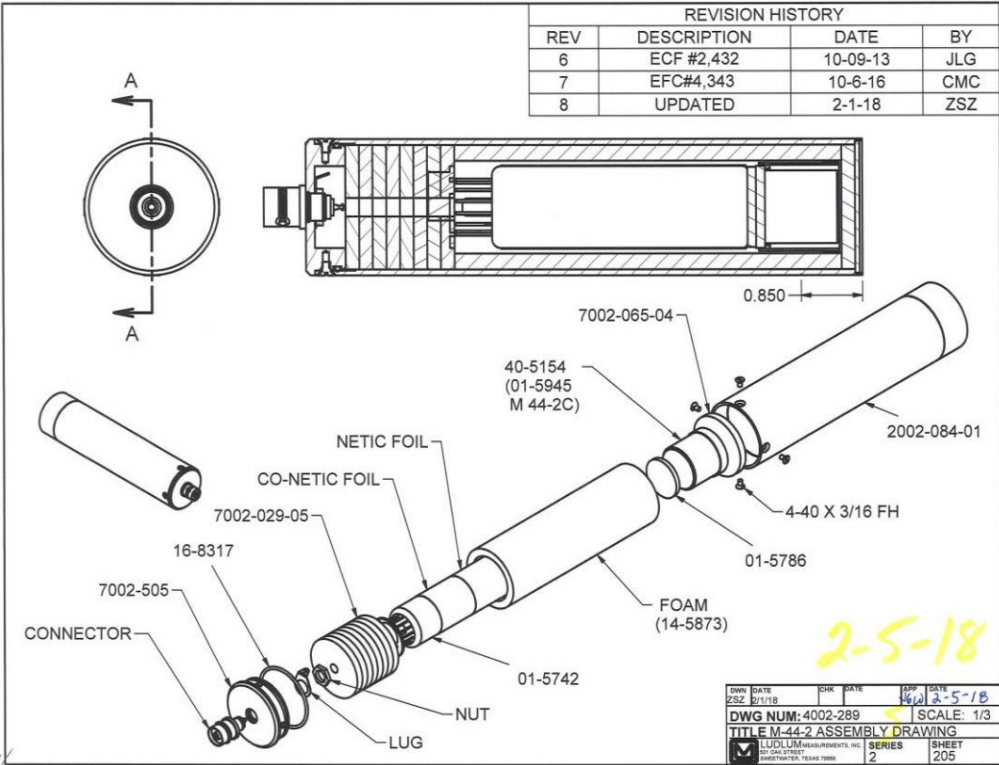
- Ludlum model 44-62 0.5x1 inch NaI detector schematic



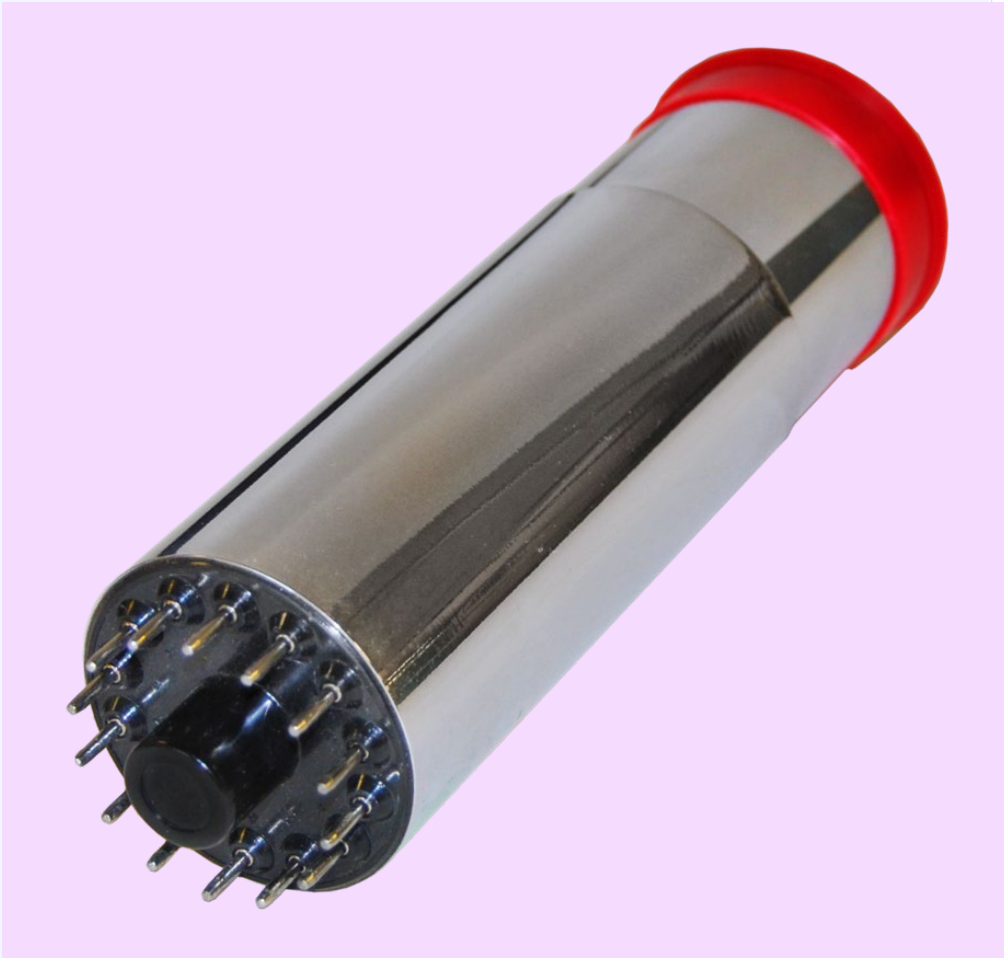
- Ludlum model [44-2](#) 1x1 inch NaI detector



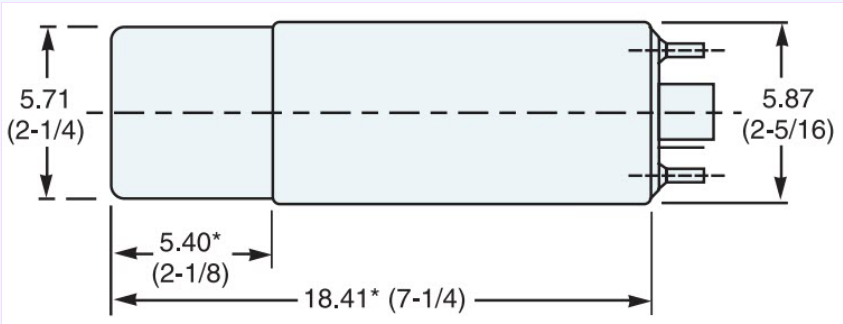
- Ludlum model 44-2 1x1 inch NaI detector schematic



- Canberra model [802-2](#) 2x2 inch NaI detector



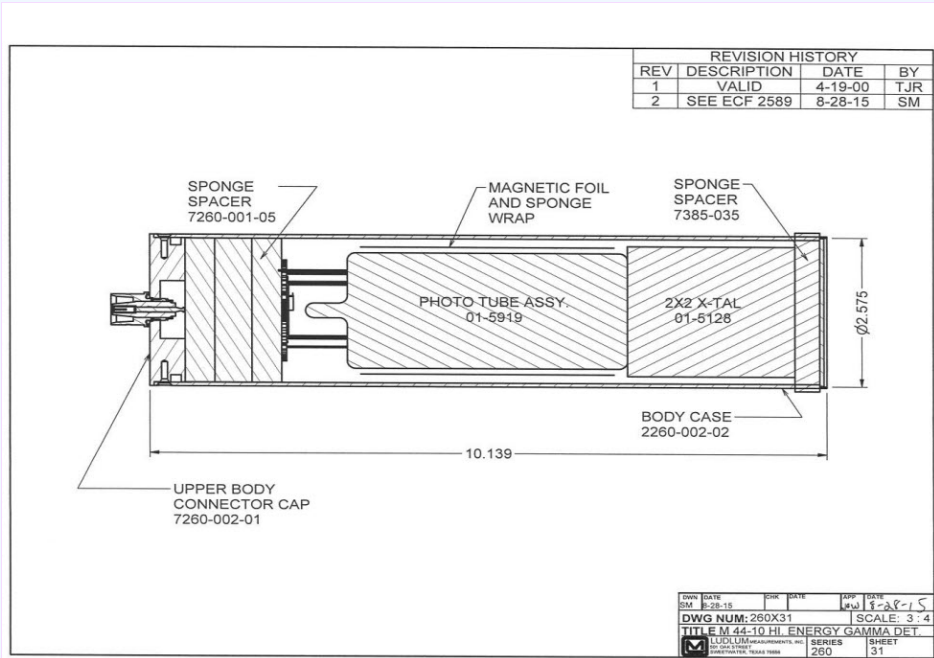
- Canberra model 802-2 2x2 inch NaI detector schematic



- Ludlum model [44-10](#) 2x2 inch NaI detector



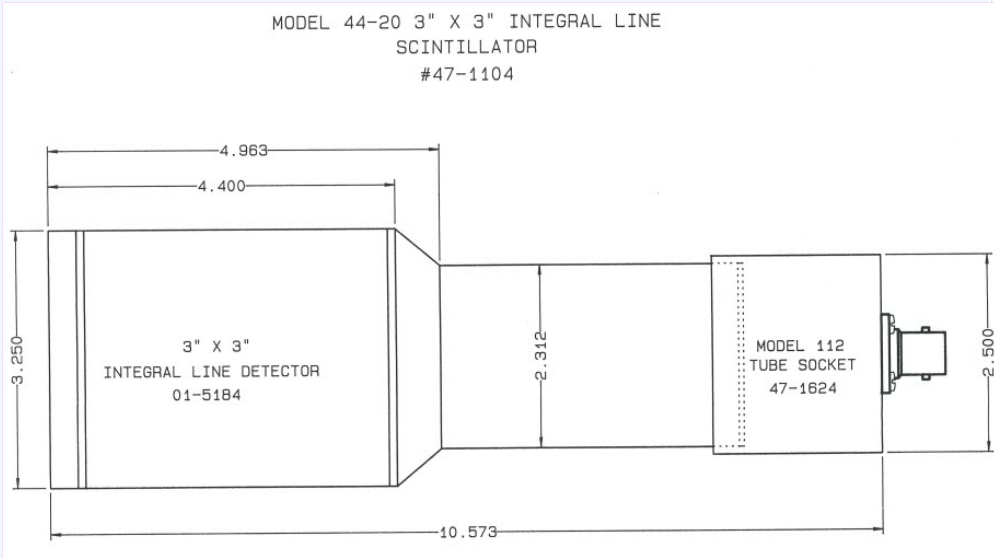
- Ludlum model 44-10 2x2 inch NaI detector schematic



- Ludlum model [44-20](#) 3x3 inch NaI detector



- Ludlum model 44-20 3x3 inch NaI detector schematic



4.4 Material Details

In this project, source data was obtained from the report published by Pacific Northwest National Laboratory, "PIET-43741-TM-963 PNNL-15870 Rev. 1 Compendium of Material Composition Data for Radiation Transport Modeling" and summarized in MCNP syntax in the table below (McConn et al., 2011). The exception is for the material definition of soil, which was taken from the Environmental Protection Agency's Federal Guidance Report 15 silty soil composition (Veinot et al., 2017).

Material	ZAID	Weight Fraction
Concrete (Regular)	1,000	-0.010000
	8,000	-0.532000
	11000	-0.029000
	13,000	-0.034000
	14,000	-0.337000
	20,000	-0.044000
	26,000	-0.014000
Soil (FGR 15)	1,000	-0.021
	6,000	-0.016
	8,000	-0.577
	13,000	-0.05
	14,000	-0.271
	19,000	-0.013
	20,000	-0.041
	26,000	-0.011
Steel (304 Stainless)	6,000	-0.000400
	14,000	-0.005000
	15,000	-0.000230
	16,000	-0.000150
	24,000	-0.190000
	25,000	-0.010000
	26,000	-0.70730

Drywall (Gypsum/Plaster of Paris)	28,000	-0.092500
	1,000	-0.023416
	8,000	-0.557572
	16,000	-0.186215
Glass (Plate)	20,000	-0.232797
	8,000	-0.459800
	11,000	-0.096441
	14,000	-0.336553
Wood (Southern Pine)	20,000	-0.107205
	1,000	-0.059642
	6,000	-0.497018
	7,000	-0.004970
	8,000	-0.427435
	12,000	-0.001988
	16,000	-0.004970
	19,000	-0.001988
	20,000	-0.001988

The following table presents densities, mass attenuation coefficients, and infinite (4) mean free path depths for discrete gamma-ray emission energies to define contamination plane radius.

Energy (MeV)	Mass Attenuation Coefficient μ/ρ (cm ² /g)	Linear Attenuation Coefficient μ (cm ⁻¹) -	Mean Free Path $1/\mu$ (cm)	Plane Radius $4/\mu$ (cm)
0.01	5.120	6.62E-03	151.05	604.22
0.02	0.778	1.01E-03	994.21	3976.84
0.03	0.354	4.57E-04	2185.97	8743.87
0.04	0.249	3.21E-04	3112.25	12449.02
0.05	0.208	2.69E-04	3718.25	14872.98
0.06	0.188	2.42E-04	4124.77	16499.10
0.07	0.177	2.29E-04	4389.09	17556.35
0.08	0.166	2.15E-04	4653.40	18613.60
0.1	0.154	1.99E-04	5018.79	20075.15
0.15	0.136	1.75E-04	5703.50	22814.02
0.2	0.123	1.59E-04	6272.47	25089.87
0.3	0.107	1.38E-04	7248.31	28993.26
0.4	0.095	1.23E-04	8099.23	32396.91
0.5	0.087	1.13E-04	8877.36	35509.42
0.6	0.081	1.04E-04	9601.43	38405.72
0.8	0.071	9.15E-05	10932.93	43731.71
1	0.064	8.22E-05	12164.13	48656.51

1.5	0.052	6.69E-05	14944.83	59779.34
2	0.044	5.75E-05	17391.39	69565.57
3	0.036	4.63E-05	21597.19	86388.74

4.5 Daughters and Chains

The CPM Calculator calculates the detector response for the primary radionuclide in one hundred to one thousand years of secular equilibrium with its daughters. This is meaningful, especially in the common case of Cs-137 (the well-known 662 keV gamma of Cs-137 is actually produced by its metastable daughter, Ba-137m). This feature can be deactivated by deselecting the check box beneath the radionuclide selection list.

The three main natural decay chain series have been truncated for use with man-made or purified radionuclides of U-238, U-235 and Th-232. For example, selecting U-238 will only include the immediate three daughters. The next sequential daughter, U-234, being so long lived, is considered a new radionuclide.

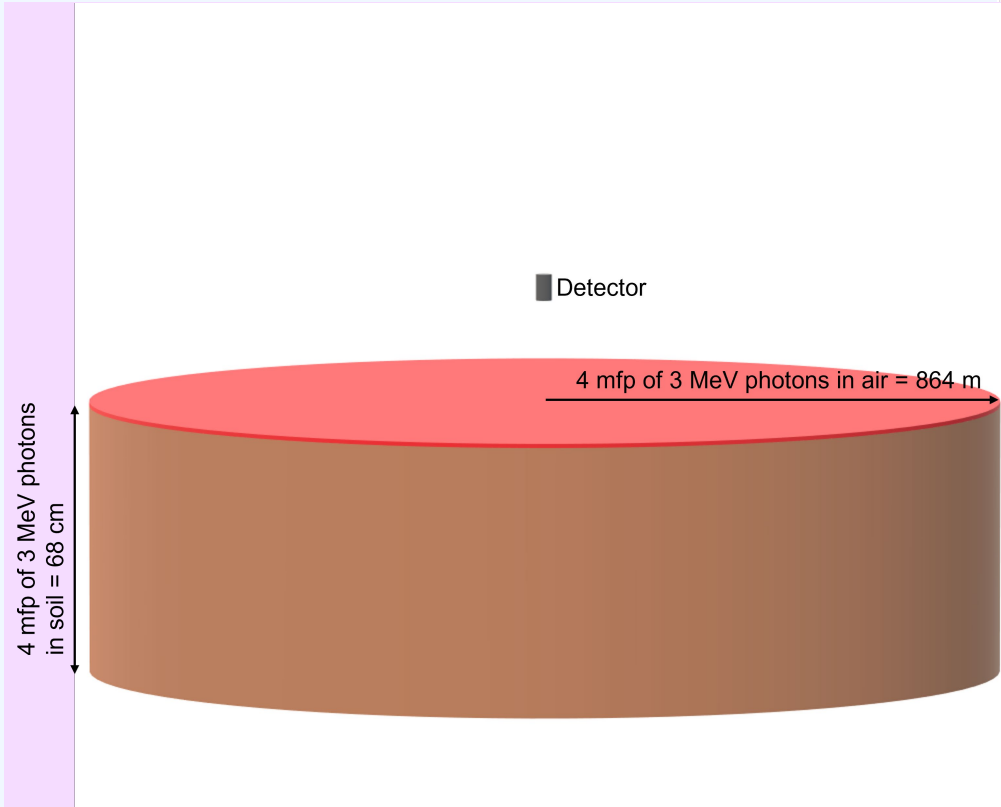
To calculate for the natural state of the above three chains, as in calculating for uranium ore, select from the radionuclide list the natural instance of the parent radionuclide, denoted by the suffix 'nat': U-238nat, U-235nat, and Th-232nat. Selecting one of these radionuclides will include the contribution of the entire natural chain.

4.6 Model Geometry and Physics

The section describes the setup of the contaminated sources and the detector geometry in MCNP/Shift.

4.6.1 Ground Plane

The geometry of the ground plane model is a 1 micron thick disc source above which a detector is suspended. The height (h) of the detector is the user's estimate of the distance in centimeters between the detector and the source of contamination. The maximum radius of the disc (R) is calculated such that the distance from the detector to the outer circumference of the circle is four mean free paths of the greatest simulated photon energy (3 MeV), a distance at which the photon is safely assumed to be attenuated.

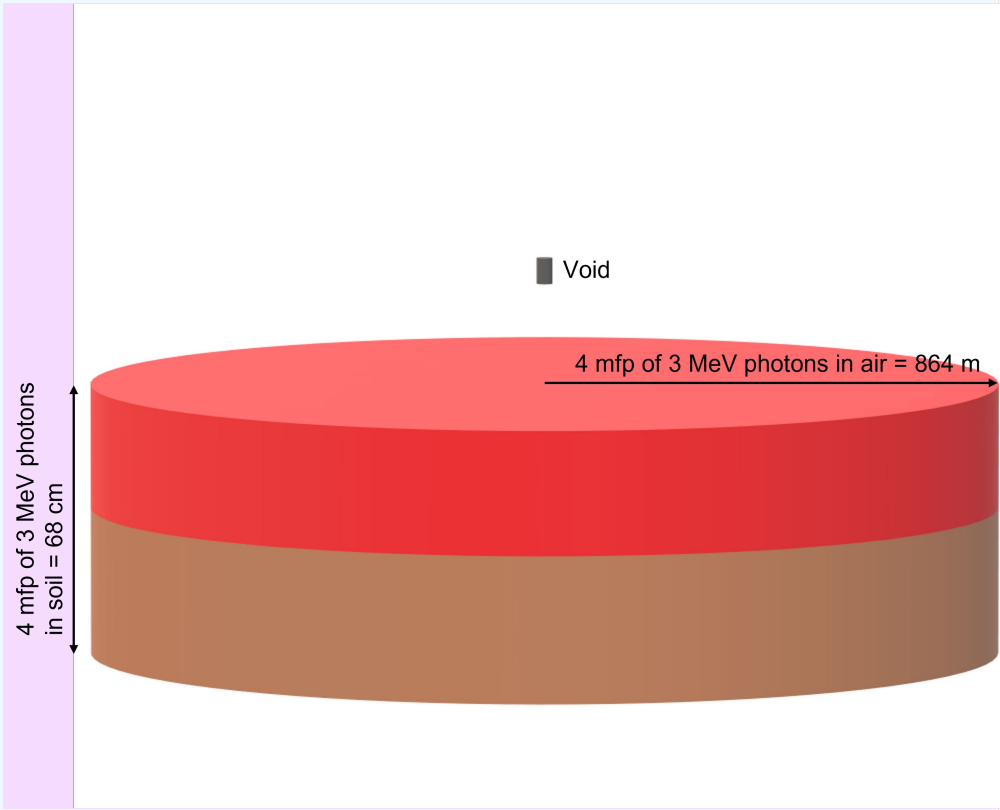


Detector responses from ground plane sources were simulated in MCNP using high performance computing clusters. Simulations were run for 19 monoenergetic photon sources using each of 120 combinations of contamination material, detector configuration, and source-detector distance. In each simulation, a pulse height tally was calculated through the NaI crystal of the modeled detector. All final MCNP F8 pulse height tally results were reported with relative errors of less than 5%.

4.6.2 Volumetric

The 6 different options for source material are soil, concrete, plate glass, wood, steel, and drywall. The model for soil, concrete, plate glass, wood, and steel is based on a uniformly contaminated cylindrical slab source of varying thickness. The average fluence through a void mimicking the geometry of a detector suspended in air at a distance above the source is calculated The geometry of the volumetric source model for all source materials

is depicted in this diagram.



Average cell fluxes for the Shift volumetric contamination runs were simulated in a high performance computing cluster. All final Shift average cell flux tally results were reported with relative errors of less than 5%.

4.7 MCNP and SHIFT Implementation

The MCNP F8 pulse-height tally may be approximated by multiplying the energy-dependent fluence by a user provided detector response function which accounts for dependencies on factors such as energy, space, and angle. See the following equation.



Detector response functions were calculated by normalizing the MCNP calculated pulse height tally for surface contamination to the Shift calculated average cell fluence for the same modeling conditions (emission energy, contamination depth, contamination material, detector configuration, and source-detector distance). See the following equation.



The detector response for monoenergetic volumetric sources was calculated as the product of the energy-binned fluence and the energy dependent response function. See the following equation.



Radionuclide-specific response:

For a given radionuclide, the detector response for each photon emission energy was interpolated from detector response of the 19 monoenergetic photon sources for the same conditions (contamination depth, contamination material, detector configuration, and source-detector distance) using PCHIP. The response at each emission energy was multiplied by the corresponding intensity of the emitted photon and the radionuclide-specific response for the given conditions was calculated as the sum of the product over all emission energies. It was assumed that photons with emission energies below 20 keV did not contribute to the response and were, therefore, omitted from the calculation.

4.8 Calculating the Activity to CPM Conversion Factor

The MCNP/Shift detector responses generated were normalized, as presented in the equation below, to obtain the i^{th} monoenergetic or radionuclide area activity to CPM conversion factor.



4.9 Calculating the Field and Target Activity in CPM

Field Activity in CPM, cpm_{FAC} , and Target Activity in CPM, cpm_{TAC} , are found by multiplying the cpm per activity conversion factor, CF, by the user's TAC in pCi/g for a radionuclide. If multiple primary radionuclides were selected, the FACs in pCi/g are also multiplied by the result. The equations for cpm_{FACi} and cpm_{TACi} for a radionuclide i may be seen below.



4.10 Calculating the Relative Fraction

The relative fraction, f_i , is the fraction of the total activity contributed by each radionuclide. The FACs are used to find the relative fractions of each radionuclide, which are then applied to the GDR. The equation for calculating the relative fraction for a radionuclide i may be seen below.



4.11 Calculating the Gross Detector Response

The GDR is the total calculated response of the detector in cpm for the desired remedial activity of the particular radionuclides in the soil. MARSSIM Equation 4-4 "Gross Activity DCGL" (U.S. EPA, 2000) is applied to find the GDR and can be seen in an edited form below.



Where f_i is the relative fraction of each radionuclide, and cpm_{TAC} is the TAC of each radionuclide in units of detector cpm.

5. Definitions of Terms and Acroynyms

Table 1 presents the definitions of the variables and their default values.

Table 1. Definitions of Terms and Acroynyms

Symbol	Definition (units)	Default	Reference
CF_i	CPM conversion factor (cpm/(pCi/g))	Isotope-specific	Calculated TAMU 2020
GDR	Gross detector response (cpm)	Isotope-specific	Calculated
FAC	Field activity concentration (pCi)	Isotope-specific	Calculated
TAC	Target activity concentration (pCi)	Isotope-specific	Calculated
f_i	relative fraction (unitless)	Isotope-specific	Calculated

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