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McSKY: A Hybrid Monte-Carlo Line-Beam Code for Shielded Gamma Skyshine Calculations

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Abstract

McSKY evaluates skyshine dose from an isotropic, monoenergetic, point photon source collimated into either a vertical cone or a vertical structure with an N-sided polygon cross section. The code assumes an overhead shield of two materials, though the user can specify zero shield thickness for an unshielded calculation. The code uses a Monte-Carlo algorithm to evaluate transport through source shields and the integral line source to describe photon transport through the atmosphere. The source energy must be between 0.02 and 100 MeV. For heavily shielded sources with energies above 20 MeV, McSKY results must be used cautiously, especially at detector locations near the source.

User Notes for
McSKY

by

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1 Summary

This program evaluates the gamma-ray skyshine dose from an isotropic, monoenergetic, point gamma-photon source collimated into either a vertical cone (i.e., silo geometry) or into a vertically oriented structure with an N-sided polygon cross section. An overhead laminate shield composed of two different materials is assumed, although shield thicknesses of zero may be specified to model an unshielded skyshine source.

The skyshine dose calculation is based on a Monte Carlo algorithm to evaluate the gamma-ray transport through the source shields and the integral line-beam method, using an improved 3-parameter approximation for the line-beam response function, to describe the subsequent transport of gamma photons through the atmosphere. The source energy may be any energy between 0.02 and 100 MeV. In the Monte Carlo shield calculation, positron transport and bremsstrahlung production are neglected, although the air transport calculation using the line-beam response function does include these components. Consequently, for heavily shielded sources with energies above about 20 MeV, McSKY results must be used cautiously especially at detector locations near the source where shield-generated bremsstrahlung may be significant.

2 Theory and Methods

The theory and validation for the methods used by McSKY are described in detail elsewhere [1, 2, 3]. In this section only a brief overview is presented.

McSKY uses a two-step hybrid method for estimating the skyshine dose arising from a shielded, monoenergetic, gamma-ray source. In this method, a Monte Carlo procedure is first used to determine the energy and angular distribution of photons escaping into the atmosphere through the source shield. These escaping photons are then treated as a bare, point, anisotropic, polyenergetic skyshine source in an infinite air medium whose subsequent transport through the air to a detector is treated by the integral line-beam response function technique [1].

2.1 Skyshine Geometries

Two skyshine geometries are available in McSKY. In the first, a point isotropic monoenergetic source is assumed to be placed on the axis of a cylindrical silo at some specified distance below the top of the silo. Placed atop the silo are one or two horizontal slab shields. The silo wall is assumed to be black so that only source photons (and secondary photons produced in the shields) that penetrate the shields can reach a detector located outside the silo.

The second McSKY geometry assumes that a point isotropic monoenergetic source is collimated vertically in such a manner that a polygonal area on the bottom of the first horizontal overhead shield is illuminated. A second slab shield may also be placed atop the first (or inner) shield. The source collimation is assumed to be ideal, that is, only photons travelling directly from the source to the illuminated area of the first shield have any possibility of penetrating the shield and contributing to the skyshine dose outside the source containment.

The use of polygonal geometry allows great flexibility in modeling realistic geometries since any illuminated area on inner surface of the shield can be approximated well by a polygon with a sufficiently large number of sides. Although McSKY assumes any polygon used to defined the source collimation is convex (i.e., all interior angles between adjacent sides are less than 180 degrees), this is not a severe restriction. Any concave polygon can be represented as sums and differences of convex polygons, so that source superposition methods [4] can be used to obtain the skyshine dose from a concave polygon as well.

2.2 The Hybrid Method

The hybrid method for shielded skyshine analyses uses first some transport model to determine the energy and angular distribution of photons that escape into the atmosphere through the source shielding. The integral line-beam method [1] is then employed to transport the escaping photons through the atmosphere to the detector. The transport model used in the first step of the hybrid method can be based on a discrete-ordinates calculation for the source shield [1, 5, 6], or on a Monte Carlo simulation for the shield [2]. It is this latter approach that is used in McSKY.

More specifically, in the hybrid method the energy and directional distribution of escaping photons is integrated over the outer surface of the source shield, and this integrated distribution is then treated as a effective point skyshine photon source whose energy and angular distribution is given by

$$S_{pt}^{eff}(E, \mathbf{\Omega}) = \int dA \, j_n(\mathbf{r}_s, \mathbf{\Omega}). \tag{1}$$

The integration is over all points $\mathbf{r}_s$ on the surface of the atmospheric side of the source shield. The leakage current j_n is related to the angular fluence Φ at the shield surface by $j_n(\mathbf{r}_s, \mathbf{\Omega}) \equiv \hat{\mathbf{n}}\cdot\mathbf{\Omega}\Phi(\mathbf{r}_s, \mathbf{\Omega})$, where $\hat{\mathbf{n}}$ is the outward unit normal to the shield surface.

With this effective point source, the skyshine dose at some point far from the source containment and at a distance x from the source can be efficiently estimated using the integral line-beam method in which the dose at x is given by

$$R(x) = \int dE \int d\Omega\, S_{pt}^{eff}(E, \mathbf{\Omega})\, \Re(x, E, \phi(\mathbf{\Omega})). \tag{2}$$

In this result $\Re(x, E, \phi)$ is the line-beam response function (LBRF) defined as the dose a distance x from a source which emits one photon of energy E in direction ϕ with respect to the source-detector axis.

For an infinite air medium of density ρ, the LBRF can be approximated by [1, 3]

$$\Re(x, E, \phi) = \kappa E(\rho/\rho_o)^2[x\rho/\rho_o]^b \exp[a - (cx\rho/\rho_o)]. \tag{3}$$

The approximation parameters a, b and c are functions of E and ϕ and κ is a constant which depends on the units used for the dose. Tabulations of a, b and c at a reference density $\rho_o = 0.0012$ g cm^{-3}, for discrete energies between 0.01 MeV to 100 MeV, and at discrete directions ϕ between 0 and 180 degrees are available [3]. For energies and directions other than those tabulated, a double interpolation scheme is used to obtain $\Re(x, E, \phi)$.

The hybrid skyshine method thus first determines from a transport calculation the effective bare skyshine source $S_{pt}^{eff}(E, \mathbf{\Omega})$. Then the skyshine dose at a specified detector location is determined by numerically integrating Eq. (2) using the infinite-air LBRF approximation of Eq. (3). The effect of the air-ground interface, which is neglected in the above procedure, is generally very small, except at small source-detector distances and for small emission angles ϕ. Recently, ground correction factors have been obtained [7] that would allow the infinite-air LBRF to be corrected for the ground interface. However, these corrections which are almost always small, have not been included in McSKY.

2.3 The Hybrid Method Used in McSKY

In McSKY, a Monte Carlo simulation is used to track photons through the overhead shields. Secondary photons from Compton scattering and annihilation of positrons produced by pair production interactions are treated. Ignored in the Monte Carlo simulation are fluorescence and bremsstrahlung, the former of little importance to skyshine because of the very low energy of fluorescence photons, and the latter producing negligible contribution for source photon energies below 20 MeV. Escaping uncollided and secondary photons that penetrate the shields are grouped by energy E and direction $\mathbf{\Omega}$, or more precisely, with respect to the angle ϕ between $\mathbf{\Omega}$ and the source-detector axis.

In the Monte Carlo phase of McSKY, photons penetrating the source shields are binned according to their energy E and their direction ϕ with respect to the source-detector axis. The energy range between 0 and E_o, the source energy, is divided into N_E contiguous equal-width subintervals whose midpoint values are denoted by E_i, $i = 1, ..., N_E$. The 180-degree range of emission directions is divided into 20 contiguous subintervals with smaller interval widths used in the more important forward (small ϕ) directions. The centroid of these angular bins is denoted by ϕ_j, $j - 1, ..., 20$. Photons leaving the outer shield surface are scored or binned as follows: (1) the number N_j^o of uncollided source photons in angular interval j (all of which have the source energy E_o), the number N_j^{pp} of uncollided annihilation photons in angular interval j (all of which have energy $E_{pp} = 0.511$ MeV), and (3) the number N_{ij}^s of secondary scattered photons with energy in energy bin i and direction in angular bin j.

Then for a simulation in which N_t source photons are tracked through the source shields, the skyshine dose, per source photon, is estimated from Eq. (3) as

$$R(x) = \frac{1}{N_t} \sum_{j=1}^{20} \left\{ N_j^o \Re(x, E_o, \phi_j) + N_j^{pp} \Re(x, E_{pp}, \phi_j) + \sum_{i=1}^{N_E} N_{ij}^s \Re(x, E_i, \phi_j) \right\}. \qquad (4)$$

2.4 Choice of Shield Materials

In McSKY, one of four materials (aluminum, concrete, iron and lead) must be specified for each of the two source shields. (A shield with zero thickness specifies that no shield is present.) Although the restriction to only four shield materials may appear somewhat limiting, extensive calculations have shown that the skyshine dose depends primarily on the *mass thicknesses* of the shields and only very weakly on the shield material itself [2]. Thus for shields with a composition other than one of the four available McSKY materials, pick the McSKY material whose atomic number is closest to that of the actual shield material and specify a mass thickness equal to that of the actual shield.

3 Required Input Data

Data may be entered (1) interactively from the keyboard, or (2) from a data input file. While modest checking of input data is attempted by McSKY, the program is not totally "bullet-proof" and the user must bear some responsibility to enter meaningful data.

NOTE: All input parameters that are lengths or distances are assumed to have units of meters except for the shield thicknesses which are units of centimeters or mean-free-path lengths.

3.1 Shield-Independent Parameters

NPTS The number of source particle histories to track through the source shields. The higher this number, the more accurate the skyshine dose should be. The total number of histories is divided into 10 batches for the purpose of estimating the errors in the skyshine doses. NPTS should be a multiple of 10.

ENERGY Energy of the photons emitted by the source (MeV). This source energy must is restricted to $0.02 \leq$ ENERGY ≤ 100 MeV.

NBE The number of equal width energy bins below the source energy that are used for the scoring of photons penetrating the overhead source shields. This number must be positive and less than or equal to 50.

MAT(1) Identification integer to specify the type of material in the first (closest to the source) horizontal slab shield above the source. Permissible values are: =1 for aluminum; =2 for concrete; =3 for iron; or =4 for lead

T(1) The shield thickness of the first (nearest the source) overhead source shield. A positive number gives the shield thickness in centimeters. A negative number gives the shield thickness in mean-free-path lengths.

MAT(2) Identification integer to specify the type of material in the second (upper) horizontal slab shield above the source. Permissible values are: =1 for aluminum; =2 for concrete; =3 for iron; or =4 for lead

T(2) The shield thickness of the second (outer) overhead source shield. A positive number gives the shield thickness in centimeters. A negative number gives the shield thickness in mean-free-path lengths.

RHOACT The air mass density in g/cm^3. The line-beam response function approximation used by McSKY assumes an air density of 0.0012 g/cm^3, but the skyshine dose is corrected to the density specified by RHOACT.

HSLAB Vertical distance (m) from the source to the bottom of the first shield (i.e., to the shield surface closest to the source). This must be positive, i.e., the source must be below the source shield.

HDET Detector elevation with respect to the source elevation (m). This elevation may be positive (to place the detector above the source) or negative (to place the detector below the source).

XSTOD The maximum horizontal distance (m) from the source at which the skyshine dose is to be evaluated. Doses will also be estimated at NDIST intermediate points, equally distributed between the source and the maximum distance XSTOD.

NDIST The number of intermediate source-to-detector distances to be used for evaluation of the skyshine dose. The intermediate distances are equally spaced between the source and the maximum distance XSTOD.

NTYPE Indicates the skyshine source geometry. Permissible values are:
=1 source is on the axis of a circular silo ("silo geometry") such that source photons are collimated into an upward cone.
=2 source is assumed to be collimated such that the illuminated area on the bottom of the first overhead shield is a convex polygon.

3.2 Geometry-Dependent Parameters

3.2.1 Silo Geometry (NTYPE = 1)

In this skyshine configuration, a point, isotropic, monoenergetic source is assumed to be on the axis of a silo with a circular cross section. The top of the silo is assumed to be in a horizontal plane and the source is below the silo top. The silo walls are assumed to be black and any in-silo scattering is ignored. The source radiation is thus collimated into an upward vertical cone whose conical angle is determined by the silo inner radius and the source elevation with respect to the silo top. The overhead source shields (if any) are assumed to be placed horizontally across the top of the silo. Only the following parameter is needed for this geometry.

ACOLL The conical half-angle of collimation for the source (in degrees). This angle must be constrained such that $0 < \text{ACOLL} < 90$.

3.2.2 Polygon Geometry (NTYPE = 2)

In this skyshine configuration, a point, isotropic, monoenergetic source is assumed to be collimated vertically such that the illuminated area on the bottom of the first shield is described by convex polygon of N sides. The polygon shape is quite arbitrary although it must be convex, i.e., all internal angles of the polygon must be less than 180 degrees.

The collimation polygon is defined by specifying the (x, y) coordinates of its N vertices. The bottom of the first overhead slab shield is taken as the $x - y$ plane with the origin taken as the intersection of this plane and the vertical through the source. The $x-$axis is directed towards the detector.

The source collimation defining this polygon is assumed to be "black" i.e., the collimation surfaces are perfect absorbers. Likewise, any radiation reflected by the overhead shields back towards the source is assumed to be absorbed. Thus the only radiation reaching the detector is that which penetrates the overhead slab shields and subsequently travels through the atmosphere.

To specify the polygon collimation for this geometry, a file name that contains the polygon data is specified in the input data file (or entered from the keyboard), i.e.,

`EDGEIN` The file name where the number of vertices of the polygon and the x, y coordinates of the vertices are to be found.

In the file `EDGEIN` the following data is needed.

`NEDGE` The number of vertices for the convex collimation polygon.

(x_i, y_i) The x, y coordinates for each of the vertices of the polygon defining the collimation of the source beam on the surface of the bottom of the source shield nearest the source. Each line contains the coordinates of one vertex, x_i followed by y_i. The vertices *must* be entered in this file in cyclic order (either clockwise or counterclockwise). It is the user's responsibility to ensure that the polygon so defined is convex.

4 Data Files

Rather than enter input data interactively with McSKY, it is often more convenient to place the input data into a separate input file and have McSKY read this file. If you indicate to McSKY that the input data is to be read from a file, McSKY will ask you to enter the file name (e.g., `MCSKY.INP`). The file will then be opened an the input data read.

The ASCII input file must contain the input data in the order specified below. The structure of an input file is thus

```
Number of histories (NPTS)
Source energy (ENERGY)
Number of energy bins (NBE)
1st shield material(MAT(1)), 2nd shield material(MAT(2))
1st shield thickness(T(1)), 2nd shield thickness(T(2))
Air density (RHOACT)
Vertical distance source to 1st shield, detector (HSLAB,HDET)
Horizontal distance from source to detector (XSTOD)
Number of intermediate source-detector distances (NDIST)
Type of collimation (1 - silo or 2 - polygon) (NTYPE)
Collimation angle or file name of vertex points (ACOLL or EDGEIN)
```

If the type of collimation is selected to be a N-sided polygon, another input ASCII file containing the coordinates of the polygon's vertices is also needed. The x, y coordinates of each vertex, in cyclic order placed one vertex per line, are placed in this second input file. The structure of this polygon definition file is as follows:

```
Number of vertices (NEDGE)
x1    y1  coordinates of vertex 1
x2    y2  coordinates of vertex 2
...
xn    yn  coordinates of vertex NEDGE
```

4.1 Example Input Files

Example input files for two cases (silo and polygon collimation) are shown below. The input parameters in the input file must appear in the order indicated. NOTE: The descriptions to the right of the data in these examples are not necessary. They are included only to provide references when examining or modifying the input file. The one exception to annotating an input data line is for the line containing the file name for the collimation polygon data. This input line must contain only the file name.

Example Input File for Silo Geometry

```
5000000            NPTS: total number source particles
20                 NBE: number of energy bins used
1.250              ENERGY: source photon energy (MeV)
2         3        MAT(1) MAT(2): shield material indices
-1.0     -2.0      T(1) T(2): shield thickness (cm)(-mfp)
0.00120            RHOACT: air density (g cm^-3)
10.00       10.00  HSLAB HDET: shield and detector heights (m)
1000.00            XSTOD: source-to-detector distance (m)
19                 NDIST: no. intermediate detector locations
1                  NTYPE: collimation type (=1 silo; =2 polygon)
30.0               ACOLL: collimation angle
```

Example Input File for Polygon Geometry

```
300000             NPTS: total number source particles
25                 NBE: number of energy bins used
6.17               ENERGY: source photon energy (MeV)
2        3         MAT(1) MAT(2): shield material indices
20.4    -0.5       T(1) T(2): shield thickness (cm)(-mfp)
0.0014             RHOACT: air density (g cm^-3)
10.0  10.0         HSLAB HDET: shield/detector height (m)
1000.0             XSTOD: max. source-detector distance (m)
9                  NDIST: no. intermediate detector locations
2                  NTYPE: collimation type (=1 silo; =2 polygon)
square.dta
```

5 Examples

Example input and output files for the two different geometries are shown below.

5.1 Silo Geometry

The first example is for silo collimation of a ^{60}Co source with two 0.5 mean-free-path shields. The first shield is concrete and the second shield is iron. Thus for the input file

```
50000                NPTS: total number source particles
20                   NBE: number of energy bins used
1.250                ENERGY: source photon energy (MeV)
2        3           MAT(1) MAT(2): shield material indices
-0.50   -0.50        T(1) T(2): shield thickness (cm)(-mfp)
0.0012               RHOACT: air density (g cm^-3)
10.00   10.00        HSLAB HDET: shield/detector height (m)
1000.0               XSTOD: source-to-detector distance (m)
9                    NDIST: no. of intermediate detector locations
1                    NTYPE: collimation type (=1 silo; =2 polygon)
30.0                 ACOLL: silo half angle of collimation
```

the following output is obtained.

```
******************* MCSKY RESULTS ********************
Number of histories                         =    50000
Source photon energy (MeV)                  =    1.250
Lower shield elevation above source (m)     =    10.00
Detector elevation above source (m)         =    10.00
Maximum source to detector distance (m)     =  1000.00

Lower (1st) Shield material = CONCRETE
Shield thickness (mfp) =      .50

Upper (2nd) Shield material = IRON
Shield thickness (mfp) =      .50


Source geometry =  SILO COLLIMATION
Collimation conical half-angle (degrees)  =    30.00
```

SKYSHINE DOSES

X(m)	g/cm^2	rad/photon	R/photon	+-%
100.00	12.00	1.16E-21	1.33E-21	1.52
200.00	24.00	2.26E-22	2.58E-22	1.70
300.00	36.00	5.57E-23	6.38E-23	1.87
400.00	48.00	1.53E-23	1.76E-23	2.05
500.00	60.00	4.51E-24	5.17E-24	2.23
600.00	72.00	1.39E-24	1.59E-24	2.44
700.00	84.00	4.44E-25	5.08E-25	2.66
800.00	96.00	1.46E-25	1.67E-25	2.91
900.00	108.00	4.92E-26	5.63E-26	3.18
1000.00	120.00	1.69E-26	1.94E-26	3.48

The first column in the above output table is the horizontal source-to-detector distance (m) while the second column gives the corresponding mass thickness $\rho_{air}x$ in units of g/cm^2. Columns 2 and 3 given the skyshine dose as air kerma and exposure, respectively. The last column gives the estimated standard deviation for both doses. It is determined by performing the Monte Carlo simulation in ten batches, using NPTS/10 particles per batch, and then calculating the standard deviation of the mean of these ten separate estimates of the dose.

5.2 N-point Polygon Geometry

The second example is for a ^{60}Co source in the center of a square building with the same horizontal source shields above the source as in the previous example. The source-to-shield and source-to-detector vertical distances are both 5 meters. The maximum source-to-detector distance is 1000 meters with 9 intermediate calculational distances. For this problem the main input data file is thus

```
50000             NPTS: total number source particles
20                NBE: number of energy bins used
1.250             ENERGY: source photon energy (MeV)
2       3         MAT(1) MAT(2): shield material indices
-0.5    -0.5      T(1) T(2): shield thickness (cm)(-mfp)
0.0012            RHOACT: air density (g cm^-3)
10.0   10.0       HSLAB HDET: shield/detector height (m)
1000.0            XSTOD: max. source-detector distance (m)
9                 NDIST: no. intermediate detector locations
2                 NTYPE: collimation type (=1 silo; =2 polygon)
square.dta
```

with auxiliary N-point polygon vertex file square.dta defined as

```
  4          NEDGE: no. of vertices
-5.0 -5.0    x-y vertex 1
 5.0 -5.0    x-y vertex 2
 5.0  5.0    x-y vertex 3
-5.0  5.0    x-y vertex 4
```

The following output is obtained.

```
******************* MCSKY RESULTS ********************
Number of histories                          =    50000
Source photon energy (MeV)                   =    1.250
Lower shield elevation above source (m)      =    10.00
Detector elevation above source (m)          =    10.00
Maximum source to detector distance (m)      =  1000.00

Lower (1st) Shield material = CONCRETE
Shield thickness (mfp) =      .50

Upper (2nd) Shield material = IRON
Shield thickness (mfp) =      .50
```

```
Source geometry = CONVEX POLYGON COLLIMATION
 4 vertices: x-y coordinates are:
    X( 1) =     -5.00     Y( 1) =      -5.00
    X( 2) =      5.00     Y( 2) =      -5.00
    X( 3) =      5.00     Y( 3) =       5.00
    X( 4) =     -5.00     Y( 4) =       5.00
```

SKYSHINE DOSES

X(m)	g/cm^2	rad/photon	R/photon	+-%
100.00	12.00	1.09E-21	1.25E-21	.70
200.00	24.00	2.14E-22	2.44E-22	.66
300.00	36.00	5.29E-23	6.06E-23	.66
400.00	48.00	1.46E-23	1.67E-23	.70
500.00	60.00	4.31E-24	4.94E-24	.78
600.00	72.00	1.33E-24	1.52E-24	.90
700.00	84.00	4.26E-25	4.88E-25	1.07
800.00	96.00	1.40E-25	1.61E-25	1.27
900.00	108.00	4.73E-26	5.42E-26	1.51
1000.00	120.00	1.63E-26	1.87E-26	1.79

6 Auxiliary Files

McSKY requires two auxiliary files, HIGHGAM.DAT and LOWGAM.DAT, to be present in the same directory as McSKY. These files contain the parameters a, b and c needed to evaluate the approximate line-beam response function of Eq. (3). The file HIGHGAM.DAT contains the parameters for gamma energies above 10 MeV, while the other file contains the parameters for gamma energies below 10 MeV. For example, the file LOWGAM.DAT begins as follows:

```
! E=     .02
      .5      -3.2260    -1.010082    .0827326
     1.5      -4.3262    -1.025872    .0829719
     2.5      -4.8423    -1.037587    .0831220
     4.0      -5.3226    -1.051969    .0832978
    .... (lines omitted)
   110.0      -8.8880    -1.413125    .0963958
   130.0      -8.9319    -1.398953    .0991899
   150.0      -8.9420    -1.382705    .1012927
   170.0      -8.9415    -1.373270    .1024275
! E=     .03
      .5      -4.4477     -.992174    .0366235
     1.5      -5.5594     -.986039    .0364442
     2.5      -6.0823     -.981497    .0363890
     4.0      -6.5680     -.977617    .0363724
     6.0      -6.9910     -.976051    .0363954
    ....
```

The line beginning with "! E= " gives the photon energy and is followed by 20 lines giving the values of a, b, and c for 20 ϕ angles at that energy. The first column is the angle ϕ (in degrees), and columns 2 through 4 give the value of a, b, and c, respectively.

From the data in these files, McSKY uses interpolation procedures to evaluate the line-beam response function at any energy between 0.02 and 100 MeV and for any emission direction between 0 and 180 degrees.

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