

THE ENSDF BASED RADIONUCLIDE SOURCE FOR MCNP

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Abstract

A utility for generating source code of the SOURCE subroutine of MCNP (a general Monte Carlo N-Particle transport code) on the basis of ENSDF (Evaluated Nuclear Structure Data File) is described. The generated code performs statistical simulation of processes, accompanying radioactive decay of a chosen radionuclide through a specified decay branch, providing characteristics of emitted correlated particles on its output. At modeling the following processes are taken into account: emission of continuum energy electrons at β^- -decay to different excited levels of a daughter nucleus; annihilation photon emission accompanying β^+ -decay; γ -ray emission; emission of discrete energy electrons resulted from internal conversion process on atomic K- and L_{I,II,III}-shells; K and LX-ray emission at single and double fluorescence, accompanying electron capture and internal conversion processes. Number of emitted particles, their types, energies and emission times are sampled according to characteristics of a decay scheme of a particular radionuclide as well as characteristics of atomic shells of mother and daughter nuclei. Angular correlations, calculated for a particular combination of nuclear level spins, mixing ratios and γ -ray multipolarities, are taken into account at sampling of directional cosines of emitted γ -rays. The paper contains examples of spectrometry system response simulation at measurements with real radionuclide sources.

Introduction

Decay of radioactive nuclei and isomeric states usually represents complex multi-stage atomic-nuclear process, at which nuclear transformations are accompanied by cascades of electromagnetic transitions in nucleus and atomic shell, resulting in emission of space and time correlated particles: photons, β -particles, discrete energy electrons, and X-rays. Correct forecasting of a detection system response at measurements with such sources requires utilization of an adequate source model that on the basis of available atomic and nuclear data would accurately reproduce peculiarities of the decay of a particular radionuclide as well as probabilistic characteristics of the decay radiations. The paper is devoted to elaboration of such radionuclide source for MCNP code [1].

Radionuclide source

General concept

At elaborating of radionuclide source a documented possibility of creating user-defined source by modifying code of the SOURCE subroutine was employed. The MCNP developers deliberately reserved this possibility to allow creating of non-standard (not foreseen by SDEF card) source. The code of the SOURCE subroutine is modified in a standard manner, i.e. by applying PATCH file. This PATCH is automatically generated by specially developed MKSOURCE utility on the basis of input data in ENSDF/2 format. As soon as PATCH is applied and SDEF card is not present in the input file, the created MCNP executable performs simulation of a decay of chosen radionuclide through the specified decay branch.

The scheme of creating of the MCNP executable is shown in fig.1. Except for the upper box the scheme corresponds to the standard procedure involving PRPR.EXE pre-processor, FSPLIT.EXE utility code and appropriate Fortran compiler.

MKSOURCE utility

The utility uses input data file in ENSDF/2 format (the extension of ENSDF data format) as a source of input information on the decay properties of a radionuclide under interest. This data file can be composed according to the known rules [2] or obtained by transforming the data of routinely updatable ENSDF evaluated nuclear data library by means of FCONV utility, developed by L.P.Ekstrom and R.B.Firestone [3]. The latter seemed to be more advantageous way and it was primary intention of this work.

On the basis of the input data the MKSOURCE utility prepares data sets, which are incorporated into the generated Fortran source code of the SOURCE subroutine. This data sets are intended for

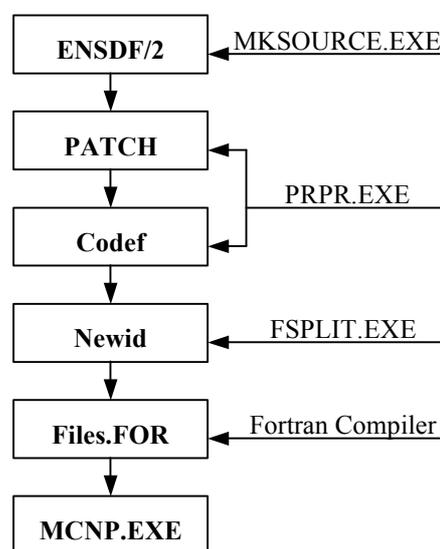


Fig.1. MCNP executable creation flowchart.

simulating of decay of a chosen radionuclide that yields random composition (quantity and types) and probabilistic characteristics (energy, time and direction of emission) of the correlated particles emitted in each accidental realization of decay.

At data set preparation the probabilities of population of different excited levels of a daughter nucleus for the considered decay branch are calculated first. Then, in case of β^- -decay, β -particle energy distribution density functions for particular energies, degrees of forbiddenness and uniqueness of β -transitions are calculated. For orbital electron capture decays the probabilities of vacancy creation on K- and L_{I,II,III}-shells are evaluated using data of the work by W.Bambinek et al. [4]. In case of β^+ -decay, probabilities of emitting of a pair of annihilation 511-keV photons are estimated assuming local deposition of kinetic energy of positron and neglecting by in-the-fly annihilation process. The first photon is emitted isotropically, and the second is emitted in the opposite direction.

Next the information about cascades of the electromagnetic transitions between excited levels of a daughter nucleus is analyzed. For each level the number of transitions, their energies, types, multipolarities, and final states are fixed. And for each transition the probability of γ -ray emission as well as the probabilities of K- and L_{I,II,III}-shell vacancy creation due to the internal conversion process are evaluated. The experimental values of internal conversion coefficients (ICC) are used for this purpose. If they are not present in the input file their values are evaluated by interpolation of the theoretical ICCs [5-7] for given energies, multipolarities and types of γ -transitions. Basing on the K- and L_{I,II,III}-shell binding energy data, energies of conversion electrons are calculated for each electromagnetic transition. Basing on the information about nuclear level spins and transition mixing ratios, angular correlation functions are calculated for each pair of cascade γ -rays using known theoretical formulas [8,9].

To ensure correct modeling of intra-atomic transitions accompanied by emission of cascade X-rays, additional data on probabilities of radiative and non-radiative atomic transitions at K- and L_{I,II,III}-shell vacancy filling are used.

Finally, a check of the correspondence of γ -ray energies to the energy difference of the nuclear levels involved into the transitions is made. Inequality of these values can reach several hundreds of electron-volts that is obviously connected with both the limited accuracy of measurements and recoil effect at γ -ray emission. A correction to the γ -ray energy is introduced when the indicated discrepancy is revealed.

Together with a PATCH file a detailed report is generated by the MKSOURCE utility on exit. The report contains detailed decay characteristics of the considered radionuclide in tabular form. Particularly, it includes branching ratios for β^\pm , ϵ and α -decays, nuclear level energies, spins, and parities, γ -transition energies, types, multipolarities, mixing ratios and ICC values, probabilities of vacancy creation on atomic shells and corresponding intensities of radiative and non-radiative atomic transition at internal conversion and electron capture processes. Also γ - γ -coincidence table is included where energies of coinciding γ -rays are indicated for each individual γ -ray.

SOURCE subroutine

The SOURCE subroutine is called at the beginning of every new history. It performs two major functions. The first one is determination of a random point inside the source where radioactive transformation is occurred. And the second one is determination of random characteristics of emitted correlated particles. The flowchart of the subroutine is shown in fig.2.

Sampling of the point inside the source is carried out on the basis of information about the source cells and volume, which contains them. This information is transferred to the subroutine through the IDUM and RDUM user data arrays, which are initialized in the input file by the corresponding cards having the same names. The utilized elements of the arrays and their assignments are indicated in table 1. Possible geometries and characteristics of the volume are shown in fig.3. The points are sampled uniformly within the specified volume, and only those ones, which fall into one of the source cells, are selected. This procedure is similar to that of the standard SDEF source, and it allows considering virtually any spatial configuration of radiation sources.

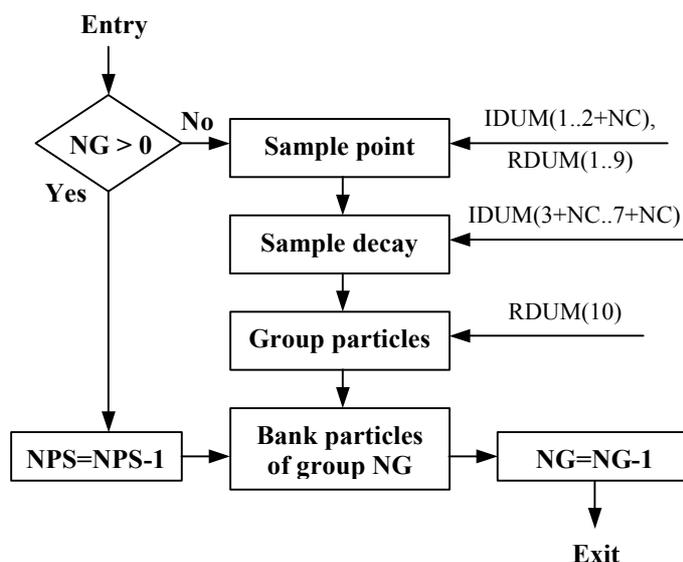


Fig.2. Subroutine SOURCE flow chart.

After the random point determination, the subroutine simulates radioactive decay processes yielding the quantity, types, energies, and directions of emission of a set of correlated particles. Depending upon the flag settings in the IDUM array (see table 1), emission of β -particles, conversion electrons, X-rays and annihilation photons, as well as γ -ray angular correlations are taken into account or ignored at decay process modeling.

The times of particle emission are sampled on the basis of the information about lifetimes of the nuclear levels involved into random realization of the sampled decay. If resolution time set in RDUM(10) is equal to zero, all particles are considered within a single history regardless of their emission times. In this case characteristics of one of the particles are assigned to XXX, YYY, ZZZ, UUU, VVV, WWW, ERG, TME, IPT, and VEL variables, while characteristics of the other particles,

Table 1. Assignments of the utilized elements of the IDUM and RDUM user data arrays.

IDUM(1)	Geometry of the volume, containing source cells (1 – parallelepiped, 2 – sphere, 3 – cylinder).
RDUM(1,2,3)	Coordinates of the volume position, $O=(X_0, Y_0, Z_0)$.
RDUM(4,5,6)	The volume dimensions ((A,B,C) – parallelepiped, $(R_1, R_2, 0)$ – sphere, (R_1, R_2, H) – cylinder).
RDUM(7,8,9)	Vector of the volume orientation, $e=(e_1, e_2, e_3)$ (cylinder only).
RDUM(10)	Resolution time, shakes (10^{-8} s)
IDUM(2)	Quantity of source cells, NC.
IDUM(3...2+NC)	Source cell numbers.
IDUM(3+NC)	β -particle flag.
IDUM(4+NC)	Conversion electron flag.
IDUM(5+NC)	X-ray flag.
IDUM(6+NC)	Annihilation photon flag.
IDUM(7+NC)	γ -ray angular correlation flag.

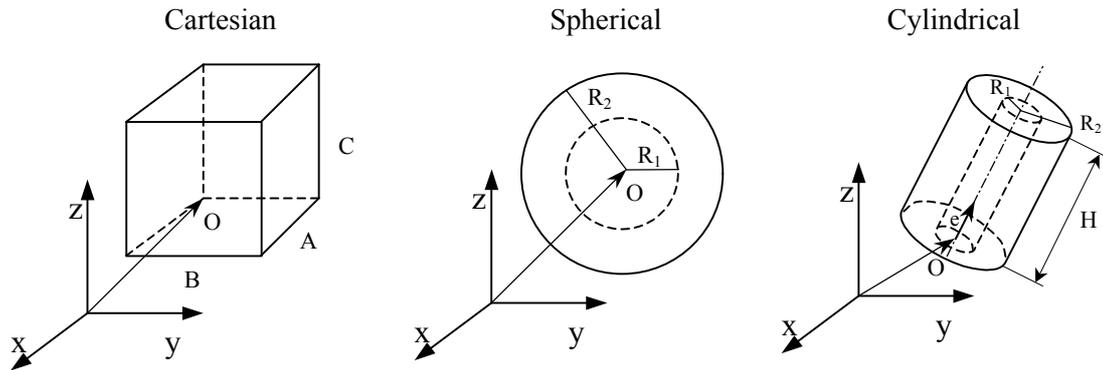


Fig.3. Geometries used at modeling of random point of particle emission.

to be considered at the same history run, are banked with help of the BANKIT subroutine. If RDUM(10) is not equal to zero, the particles are grouped into time intervals of the specified resolution time length. After this each particle group is considered independently of each other in separate history runs. At that the NPS particle counter is not incremented ensuring normalization of the final results per one decay of the parent nucleus though the considered decay branch.

Examples of spectrum modeling for measurements with real radionuclide sources

Let us consider examples of application of the described approach to modeling of ^{60}Co and ^{137}Cs radionuclide source radiation spectra at measurements with HPGe detector. In both cases the same hypothetical broad-energy detector like GAMMA-X (Ortec) or BEGe (Canberra) will be considered. The detector model is shown in fig.4. The sensitive volume of the detector has cylindrical shape with dimensions $\text{Ø}80 \times 30$ mm that approximately corresponds to the detector with 50% of relative efficiency at 1332.5 keV. The detector input window is 0.5 mm thick beryllium. Inactive germanium layer thickness from the input window side is $0.3 \mu\text{m}$. The detector design components on the backside of the Ge crystal are simulated by 20 mm aluminum layer. The case of a point source located on the detector axis of symmetry at 5 mm distance from its input window is considered. The resolution time of 500 ns is chosen for being typical value of the pulse pair resolution time of regular pile-up rejector circuits.

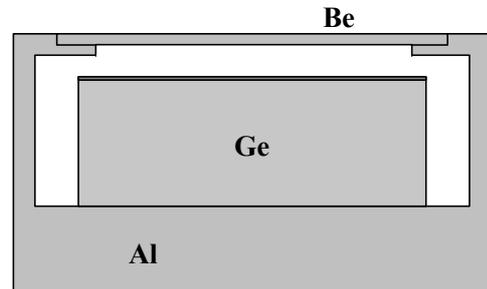


Fig.4. Detector model.

^{60}Co radiation spectra, simulated in two different approaches, are shown in fig.5. In the first approach the standard SDEF card source, emitting equal intensity 1173.2 and 1332.5 keV γ -rays, was used. Events accumulated in the tally 8 energy bins were multiplied by a factor of 2 with use of FM card for taking into account emission of two gammas per one decay of ^{60}Co . In the second approach the developed ENSDF based radionuclide source was used with β -particle emission and γ -ray angular correlations enabled.

One can see significant difference of the calculated spectra all over the energy range that is due to

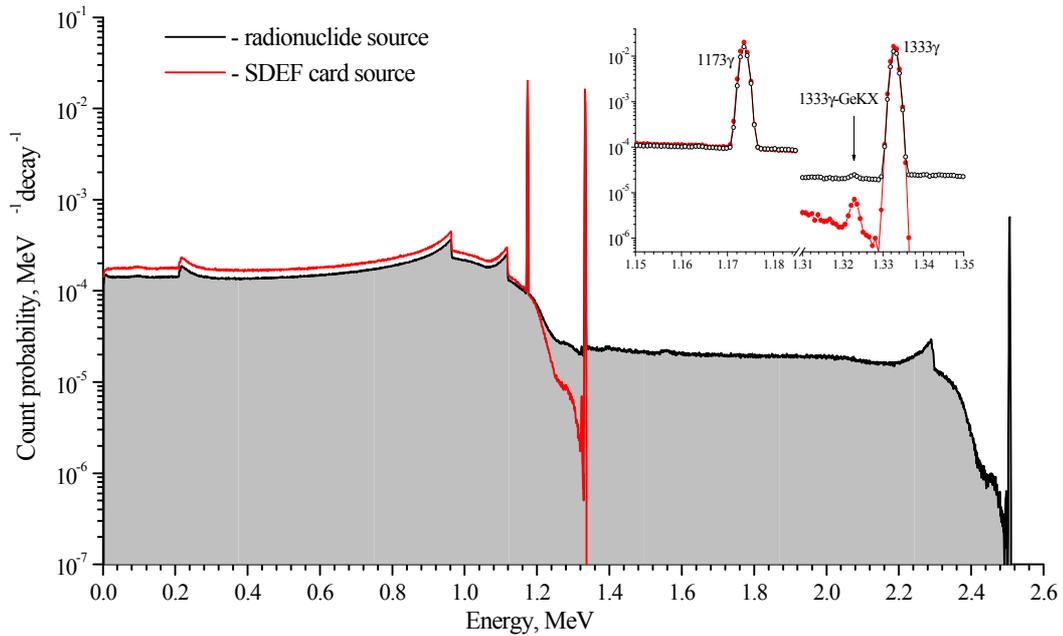


Fig.5. ^{60}Co source radiation spectra simulated with use of standard (SDEF card) and developed ENSDF based radionuclide sources.

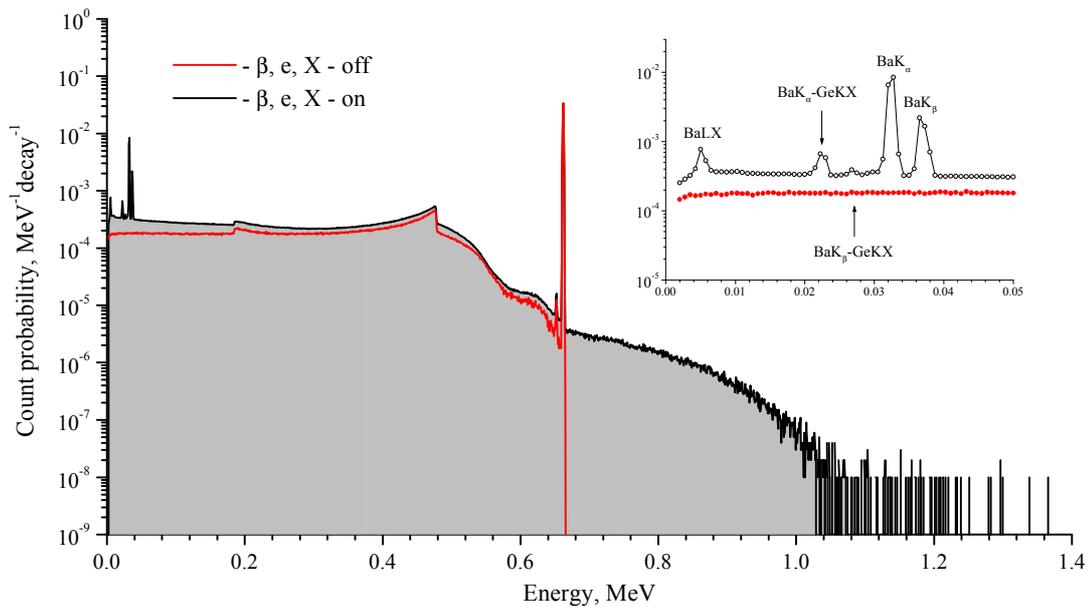


Fig.6. ^{137}Cs source radiation spectra computed with use of developed ENSDF based radionuclide source in two different modes of simulation.

the so-called true-coincidence summing effect. This effect causes transfer of compton continuum and full energy peak events into the higher energy region. For the case considered, 1173.2 and 1332.5 keV full energy peak areas are decreased by 20% due to the effect, which is more than significant for the quantitative γ -spectrometry measurements.

Spectra simulated for the case of ^{137}Cs source are shown in fig.6. The calculations were made

with use of ENSDF based radionuclide source in two simulation modes – with and without taking into account β -particle, conversion electron and X-ray emission. The differences of the calculated spectra are noticeable all over the energy range that is due to the registration of high-energy β -particles ($E_1^{\max} = 514.0$ keV, $E_2^{\max} = 1175.6$ keV) and Ba X-rays. In the X-ray region of the spectrum, which is shown separately, Ge KX-ray escape peaks are present in addition to the K and LX-ray peaks of Ba.

Conclusions

The MKSOURCE utility was created for automatic PATCH file generating for the MCNP code, extending its suit of radiation sources. The main component of the PATCH is the source code of the SOUCRE subroutine, which contains a complete set of data required for correct simulating of radioactive decay process of the selected radionuclide. This data set is created on the basis of routinely updatable ENSDF evaluated nuclear data library. The SOUCRE subroutine performs full-scale imitation of random realizations of decay to determine accidental characteristics of correlated photons, X-rays, β -particles and internal conversion electrons. It makes it possible to apply MCNP code for simulating response of detection systems, including coincidence and anti-coincidence spectrometers, at measurements with real radionuclide sources.

As one of the possible applications of the developed approach, the problem of the true-coincidence correction factor evaluation, being one of the vital problems in γ -, β - and X-ray spectrometry [10-12], can be mentioned. Application of MCNP to the problem with utilization of the elaborated ENSDF based radionuclide source has recently shown promising results [13].

The major weak point of the elaborated approach is necessity of creation of the MCNP executable each time when switching to another radionuclide. Presently a new version of the MKSOURCE utility is developed, which is aimed on transferring of all required data to the SOURCE subroutine through the input file. In such approach the MCNP executable containing modified SOURCE subroutine code must be created only once in the very beginning.

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