The event generator DECAY4 for simulation of double beta processes and decay of radioactive nuclei

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Abstract

The computer code DECAY4 is developed to generate initial energy, time and angular distributions of particles emitted in radioactive decays of nuclides and nuclear (atomic) deexcitations. Data for description of nuclear and atomic decay schemes are taken from the ENSDF and EADL database libraries. The examples of use of the DECAY4 code in several underground experiments are described.

1 Introduction and overall description of the DECAY4

Despite the fact that effect to background ratio is the central problem of all experimental physics, there is a certain class of experiments for which this problem is so crucial that even the possibility of their performance itself depends strongly on the reached background level of the used detectors. These are so called underground experiments devoted to investigation of the very rare or forbidden decays and processes like, for instance, double beta decay, proton decay, dark matter particles search, solar neutrino study and so on. The ultimate sensitivity of such experiments is determined mainly (except the available source strengths) by the detector background. The first origin of background is due to cosmic rays and can be eliminated by the proper underground site for the set up. The second (and the most crucial for sensitivity) source of the background is the decays of the nuclides from the radioactive impurities in the detector itself, in the materials used for detector mounting and shielding, and in the surroundings. Therefore it is obvious that simulation of the background and, in particular, simulation of the nuclides decays is the overwhelmingly important part of such kind of research which can allow: i) to understand and determine the origins of the background and hence to find certain methods to eliminate or suppress the background contributions; ii) to build up the background model and response functions of the detector for the effect being sought (together with the detector energy and efficiency calibrations, resolution, source activities, etc.), thus to extract and evaluate searched effect (or to exclude it) more precisely.

There are several general programs, which are commonly used for simulation of the particles interactions in the experimental set up as, for example, GEANT package [1] or EGS4 code [2]. In any such a program user should describe initial kinematics of events by using the so called event generator. The last is an important part of the simulation program providing the information, which particles and how many of them are emitted, what are their energies, directions of movement and times of emission. Existing computer codes RADLST [3] and IMRDEC [4] only determine the radiation spectra due to decay of nuclides, and therefore could not be used for the further particles tracking.

In attempt to cover this lack, the code, named DECAY4, was developed for generation of events in the low energy nuclear and particle physics (double beta decay and decay of radioactive nuclides). This code was elaborated during the last decade, mainly for 2β decay research [5]. The plan of the paper is as following: first, the overall features of the DECAY4 generator and used databases are considered, then detail descriptions of the parts associated with the double beta decay of atomic nuclei and decays of the natural and artificial radioactive nuclides are presented. In the last section several examples illustrating the use of the DECAY4 generator in the real underground experiments are shown.

The developed program DECAY4 gives the possibility to generate events of the 2β decay of atomic nuclei and of the radioactive decays (α, $\beta^{\pm}$, p, n decay, electron capture) of all known unstable isotopes. It is divided into two main sections:

a) INIT – search and reading of all parameters of the nucleus and its decay needed for decay simulation from the ENSDF [6] (or NuDat [7]), EADL [8] and other libraries, in order to build up the nuclear and atomic decay schemes;

b) GENDEC – a Monte Carlo events generator itself.

The ENSDF database library includes the following information on about 2500 isotopes used for generation of the radioactive decays: a) decay modes, their probabilities and energy releases, isotopes half-lives; b) radiation type, particles energies and intensities; c) parameters of nuclear levels (half-life, spin, parity and excitation energy); d) parameters of nuclear transitions (branching ratios, multipolarities, coefficients of internal conversion and mixing ratios).

The DECAY4 code uses also tables with the data on atomic properties of isotopes (electron binding energies, electron capture (EC) subshell ratios, X rays and Auger electrons intensities) from the EADL database [8] (as well as from [9]) and tables with theoretical Hager-Seltzer conversion coefficients [10].

The GENDEC part of the DECAY4 generates the energy, time of emission, direction and polarization for the following emitted particles: 1) electrons and positrons from single and double β decay; 2) α particles from α decay, protons and neutrons from p and n decays; 3) γ quanta from nuclear deexcitation process; 4) conversion electrons; 5) e^-e^+ pairs from the internal pair conversion; 6) γ quanta from bremsstrahlung in β decay and EC; 7) neutrinos (antineutrinos) from EC or β (2β) decay; 8) X rays and Auger electrons from the atomic deexcitation process.

2 Double beta decay processes

The DECAY4 describes double beta processes ($2\beta^-$ and $2\beta^+$ decays, electron capture with emission of positron $\varepsilon\beta^+$ and double electron capture 2ε) for all nuclides. 2β transitions to the ground state as well as to excited 0^+ and 2^+ levels of the daughter nucleus are allowed. If 2β decay occurs to an excited level of a nucleus, the electromagnetic deexcitation process follows. The energy release $Q_{\beta\beta}$ for double beta processes is taken from the table of the atomic masses [11]. For each transition to the ground or an excited level, various modes (with emission of two neutrinos or Majoron, neutrinoless decays due to nonzero neutrino mass or right-handed admixture in the weak interaction, etc.) and mechanisms (two-nucleon $2n$ and Δ-isobar N*) of double beta decay are possible. Below we give the list of double beta processes which could be simulated with the DECAY4:

1. $0\nu2\beta^{\pm}$ decay with neutrino mass, $0^+ - 0^+$ transition, $2n$-mechanism;
2. $0\nu2\beta^{\pm}$ decay with right-handed currents, $0^+ - 0^+$ transition, $2n$-mechanism;
3. $0\nu2\beta^{\pm}$ decay with right-handed currents, $0^+ - 0^+$ and $0^+ - 2^+$ transitions, N*-mechanism;
4. $2\nu2\beta^{\pm}$ decay, $0^+ - 0^+$ transition, $2n$-mechanism;
5. $0\nu2\beta^{\pm}$ decay with emission of Majoron, $0^+ - 0^+$ transition, $2n$-mechanism;

6. $0\nu2\beta^{\pm}$ decay with double Majoron emission, $0^+ - 0^+$ transition, $2n$-mechanism; decay with charged $L = -2$ Majoron or massive vector Majoron;

7. $0\nu2\beta^{\pm}$ decay with right-handed currents, $0^+ - 2^+$ transition, $2n$-mechanism;

8. $2\nu2\beta^{\pm}$ decay, $0^+ - 2^+$ transition, $2n$- and N*-mechanisms;

9. $0\nu\varepsilon\beta^+$ decay;

10. $2\nu\varepsilon\beta^+$ decay, $0^+ - 0^+$ and $0^+ - 2^+$ transitions;

11. $0\nu2\varepsilon$ decay;

12. $2\nu2\varepsilon$ decay, $0^+ - 0^+$ and $0^+ - 2^+$ transitions.

The theoretical formulae for the energy and angular distribution $\rho(E_1, E_2, cos\theta)$ of emitted electrons or positrons are based on works [12, 13, 14, 15, 16]. For example, for the first process:

$$\rho(E_1, E_2, cos\theta) = p_1(E_1 + 1)F(E_1, Z)\; p_2(E_2 + 1)F(E_2, Z)\delta(E_0 - E_1 - E_2)(1 - \beta_1\beta_2 cos\theta), \quad (1)$$

where E_i is the kinetic energy of the i-th e$^-$ or e$^+$ (in units of the electron mass m_ec^2), p_i is the momentum (in units of m_ec), $F(E_i, Z)$ is the Fermi function, Z is the atomic number of the daughter nucleus ($Z > 0$ for $2\beta^-$ and $Z < 0$ for $2\beta^+$ decay), θ is the angle between the particles directions, E_0 is the energy available for the particles ($E_0 = Q_{\beta\beta} - E_j^{ex}$ for $2\beta^-$ decay and $E_0 = Q_{\beta\beta} - 4 - E_j^{ex}$ for $2\beta^+$ decay, E_j^{ex} is the energy of the populated level of the daughter nucleus), $\beta_i = p_i/(E_i + 1)$.

3 Radioactive decays of nuclides

The DECAY4 describes six decay modes: β^-, α, p and n decays, electron capture and β^+ decay (EC) and isomeric transition (IT). The modes d ($d = \beta^-$, α, p, n, EC, IT), their probabilities p^d, available decay energies Q^d and isotopes half-life $T_{1/2}$ are taken from the ENSDF [6] or NuDat [7] databases. The decay mode d is sampled according to the probabilities p^d.

β^- **decay.** The endpoint energies in β^- decay E_i^0 are related with the energy release Q^{β^-} and the level energies E_i^{ex} of the daughter nucleus by the equation

$$Q^{\beta^-} = E_i^0 + E_i^{ex}. \quad (2)$$

Kinetic energy of the beta particle E is sampled in accordance with the distribution

$$\rho(E) = p \cdot (E + 1) \cdot \left(E_i^0 - E\right)^2 \cdot F(E, Z) \cdot S_k(E), \quad (3)$$

where $S_k(E)$ is the factor of forbiddenness. Probability of the internal bremsstrahlung in beta decay and energy-angular distribution of bremsstrahlung γ quanta are calculated as in [17].

α, **p, n decays.** The energies of particles E_i^k ($k = \alpha, p, n$) are related with the level energies E_i^{ex} of the daughter nucleus by the equation

$$E_i^k = A_d/A_p \cdot (Q^k - E_i^{ex}), \quad (4)$$

where A_p, A_d is the mass numbers of the parent and daughter nuclei, respectively.

EC (electron capture and β^+ decay). The ENSDF database includes the information on the probabilities p_i^{EC} (for EC) and $p_i^{\beta^+}$ (for β^+ decay) for i-th level of the daughter nucleus. If the level is populated in β^+ decay, energy of positron is sampled according to (3), where

$$E_i^0 = Q^{EC} - 2 - E_i^{ex}. \quad (5)$$

If the i-th nuclear level was populated in the electron capture, the number of the atomic subshell x ($x = K$, L_1, L_2, L_3, M_1, M_2, ..., M_5, N_1, N_2, ..., N_7, O_1, O_2, ..., O_7), where primary electron vacancy is created, is sampled according to probabilities P_x^{EC} [9]:

$$P_x^{EC}(Z, q_x) = const \cdot n_x p_x^{2(k_x-1)} q_x^{2(L-k_x+1)} \beta_x^2 B_x / [(2k_x - 1)!(2L - 2k_x + 1)!], \tag{6}$$

where L is the electron capture transition angular momentum, n_x is the relative occupation number for partially filled subshells x ($n_x = N_x/N_x^{\max}$, N_x is the number of electrons in the subshell x, $N_x^{\max}$ is the maximal number of electrons in the subshell), $q_x = Q^{EC} - E_i^{ex} - E_x$ is the neutrino energy, E_x is the electron binding energy in the parent atom, and k_x is x subshell angular momentum. The squared amplitudes $\beta_x^2 B_x p_x^{2(k_x-1)}$ of the bound-state electron radial wave functions and the electron binding energy E_x are taken from [18, 9]. The internal bremsstrahlung probability and spectra of bremsstrahlung γ quanta in allowed electron capture transition from x atomic subshell is calculated in accordance with [18].

Nuclear deexcitation process. The nuclear deexcitation process occurs if a daughter nucleus is in the excited i-th level with energy E_i^{ex}. The electromagnetic transition from i-th to j-th level is sampled according to probabilities

$$p_{ij} = J_{ij} / \sum\nolimits_j J_{ij}, \tag{7}$$

where J_{ij} is the branching ratio of electromagnetic transition from i-th level to j-th taken from the NuDat or ENSDF databases.

There are three possible modes of electromagnetic transition with emission of: (1) γ quantum with energy $E^\gamma = E_i^{ex} - E_j^{ex}$; (2) conversion electron with energy $E_x^{ce} = E_i^{ex} - E_j^{ex} - E_x$ (the condition $E_x^{ce} > 0$ should be fulfilled), here E_x is the electron binding energy on the x subshell; (3) conversion electron-positron pair with total energy $E^{cp} = E_i^{ex} - E_j^{ex} - 2$ (if $E^{cp} > 0$). To sample the mode, the respective probabilities p_{ij}^γ, p_{ij}^{ce}, p_{ij}^{cp} are used, where

$$p_{ij}^\gamma = 1/(1 + \alpha_{ij}^{ce} + \alpha_{ij}^{cp}),\ p_{ij}^{ce} = \alpha_{ij}^{ce} p_{ij}^\gamma,\ p_{ij}^{cp} = \alpha_{ij}^{cp} p_{ij}^\gamma \tag{8}$$

for all transitions beside E0,

$$p_{ij}^\gamma = 0,\ p_{ij}^{ce} = 1/(1 + I_{ij}^{cp}/I_{ij}^{ce}),\ p_{ij}^{cp} = I_{ij}^{cp}/I_{ij}^{ce} \cdot p_{ij}^{ce} \tag{9}$$

for E0 transition, where α_{ij}^{ce}, α_{ij}^{cp} are the coefficients of the internal electron and pair conversion, respectively, and I_{ij}^{ce}, I_{ij}^{cp} are the intensities of internal electron and pair conversion, respectively.

Total α_{ij}^{ce}, partial subshell $\alpha_{ij}^{ce}(s_m)$, shell $\alpha_{ij}^{ce}(s)$ coefficients of electron internal conversion is related by

$$\alpha_{ij}^{ce} = \sum\nolimits_s \alpha_{ij}^{ce}(s);\ \alpha_{ij}^{ce}(s) = \sum\nolimits_m \alpha_{ij}^{ce}(s_m), \tag{10}$$

where s is the shell index and m is the subshell index of the s shell ($s_m \equiv x$). Coefficients α_{ij}^{ce} and $\alpha_{ij}^{ce}(s)$ are taken from the NuDat or ENSDF databases. In case if their values are absent, the coefficients are calculated as

$$\alpha_{ij}^{ce}(s_m) = [\alpha_{ij}^{ce}(s_m, E^\gamma, \pi_1\lambda_1, Z) + \delta_{ij}\alpha_{ij}^{ce}(s_m, E^\gamma, \pi_2\lambda_2, Z)]/(1 + \delta_{ij}^2), \tag{11}$$

where the values of partial coefficients $\alpha^{ce}(s_m, E^\gamma, \pi\lambda, Z)$ are taken from [10]. Here $\pi\lambda$ is transition multipolarity, and δ_{ij} is the mixing ratio of different multipolarities in the $i \to j$ transition. For pure $E0$ transitions, electron conversion coefficients are calculated according to formulae from [9]. Coefficient of internal pair conversion α_{ij}^{cp} is given by formulae similar to (10), and partial coefficients $\alpha^{cp}(E^{\gamma},\pi\lambda,Z)$, and electron-positron energy and angular distributions are calculated according to formulae from [9, 19].

X rays and Auger electrons. The vacancies in the atomic shells are created in the electron capture or in the result of internal electron conversion. Ionized atom is deexcited filling the vacancies by electrons from higher atomic shells; X rays and Auger electrons are emitted in this process. For the sampling of the atomic deexcitation process, the values of the electron binding energies and occupation numbers, radiative and radiationless partial widths are taken from the EADL library [8]. The type of process (radiation or Auger electron emission) is sampled accordingly to the values of radiative and radiationless partial widths. For the vacancy in the s_i subshell, the energy of X ray for radiative process, in which higher vacancy q_j is created, and the energy of Auger electron for nonradiative process (vacancies q_j and t_l are created) are given by

$$E^X_{s_i-q_j} = E_{s_i}(Z) - E_{q_j}(Z);\ E^A_{s_i-q_jt_l} = E_{s_i}(Z) - E_{q_j}(Z) - E_{t_l}(Z) - \Delta E_{q_jt_l}. \tag{12}$$

Correction $\Delta E_{q_jt_l}$ is found from equations in [20]. Multivacancy corrections for energies and partial widths are included also. The X ray and Auger electron energy spreading is accounted according to Lorentzian distribution function [20].

Decay chains and time characteristics. Time interval T^k between appearance of the unstable state k of the nucleus or atom and its decay with emission of the particle is sampled in accordance with the relation

$$T^k = -T^k_{1/2}\ln\eta/\ln 2, \tag{13}$$

where η is a random number uniformly distributed in the range $(0,1)$, $T^k_{1/2}$ is a half-life of the unstable state. The DECAY4 can also simulate the full decay chain of the parent nuclide together with its daughters. As an example, the generated spectra of particles, emitted in decay of nuclides from full ^{238}U chain, are shown in fig. 1. Activities of all daughter nuclei are calculated by the DECAY4.

Angular correlations between emitted particles. The direction (polar and azimutal angles θ_i, φ_i) of the particle i is sampled as isotropical if one of the next conditions is fulfilled: 1) the particle is the first in the decay of unoriented parent nuclear state i; 2) $I_i < 1$ (I_i is nuclear spin before emission of the particle i); 3) $T^i > \tau_{\max}$ (T^i is the time given by (13), $\tau_{\max}$ is user defined parameter (time) to account the influence of external fields which violate the angular correlation); 4) $\lambda_i = 0$ or $\lambda_{i-1} = 0$ (λ_i and λ_{i-1} are angular momenta of particles i and $i-1$, if particle $i-1$ exists); 5) one of the values I_{i-1}, I_i, I_{i+1}, λ_i, λ_{i-1} is unknown and could not be evaluated. In case, if particle $i+1$ does not satisfy any of the above conditions but particle i satisfies one of them, the polar angle θ^i_{i+1} of particle $i+1$ in the coordinate system of particle i is sampled in according to correlation function [21]

$$W(\theta^i_{i+1}) = \sum\nolimits_{k_{i+1}=0}^{k^{\max}_{i+1}} A^-_{k_{i+1}}(\lambda_i\lambda'_iI_{i+1}I_i,x_i)A^+_{k_{i+1}}(\lambda_{i+1}\lambda'_{i+1}I_{i+2}I_{i+1},x_{i+1})P_{k_{i+1}}(\cos\theta^i_{i+1}), \tag{14}$$

where $\lambda'_i = \lambda_i \pm 1$ is the second possible angular momentum of the particle (for the mixture of multipolarities), x_i is type of the particle i ($x_i = \gamma$, β, α, e), $A^{\pm}_{k_{i+1}}(\lambda_i\lambda'_iI_{i+1}I_i,x_i)$ are angular momenta functions, and k is even. In this case correlation function is independent from the azimutal angle φ^i_{i+1}. If the next emitted particle $i+2$ exists, which does not satisfy any condition among 1)–5), its direction is determined by the more complicated correlation function, which depends on directions of previous particles. Correlation of linear polarisations of γ quanta is also taken into account [21].

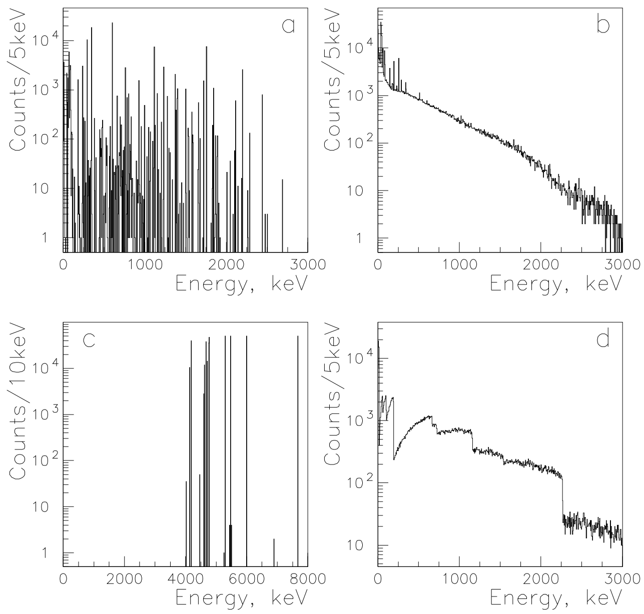

Figure 1: Generated initial energy spectra of particles emitted in the decay of ^{238}U chain (in equilibrium): (a) γ quanta, (b) electrons, (c) α particles, (d) antineutrinos.

4 Conclusions

The code DECAY4 was successfully used in several underground experiments for detectors design and optimization, simulation of the backgrounds (with the help of the GEANT package) and for evaluation of the results. Some examples are listed below.

1. Kiev 2β decay experiments performed in the Solotvina Underground Laboratory in a salt mine 430 m underground ($\simeq$1000 m w. e.):

1.1. Cadmium tungstate crystal scintillators (enriched in ^{116}Cd to 83%) were used to study ^{116}Cd [22, 23]. The background of the $^{116}CdWO_4$ crystal (15.2 cm^3) in the energy region of interest ($Q_{\beta\beta}$=2805 keV) was equal to $\approx$0.6 counts/y·kg·keV. With the 19175 h statistics the half-life limit for neutrinoless 2β decay of ^{116}Cd was set: $T_{1/2}^{0\nu} \geq 3.2 \cdot 10^{22}$ y (90% C.L.) [23]. Limits on 0ν modes with emission of one (M1) or two (M2) Majorons were established also: $T_{1/2}^{0\nu M1} \geq 1.2 \cdot 10^{21}$ y and $T_{1/2}^{0\nu M2} \geq 2.6 \cdot 10^{20}$ y (90% C.L.) [24]. Comparing these limits with the theory, the restrictions on the neutrino mass $\langle m_\nu \rangle \leq 3.9$ eV and Majoron-neutrino coupling constant $g \leq 2.1 \cdot 10^{-4}$ were derived, which are among the most sensitive results for other nuclei [16].

1.2. The study of the 2β decay of ^{160}Gd was carried out with the help of the 95 cm^3 Gd_2SiO_5:Ce crystal scintillator. The background was reduced to $\approx$1.0 cpd/keV·kg in the vicinity of $Q_{\beta\beta}$ energy ($\approx$1.73 MeV). The improved half-life limit was set for $0\nu2\beta$ decay of ^{160}Gd: $T_{1/2}^{0\nu} \geq 1.2 \cdot 10^{21}$ y at 68% C.L. [25].

2. DAMA collaboration experiments performed deep underground in the Gran Sasso National Laboratory:

2.1. Two radiopure CaF_2:Eu crystal scintillators (370 g each) have been used to study 2β decay of ^{46}Ca and double electron capture of ^{40}Ca as well as for dark matter search. The highest up-to-date half-life limits were reached for 0ν and 2ν double electron capture of ^{40}Ca: $T^{0\nu}_{1/2} \geq 4.9\cdot10^{21}$ y and $T^{2\nu}_{1/2} \geq 9.9\cdot10^{21}$ y (68% C.L.) [26].

2.2. The study of the $2\beta^+$ decay of ^{106}Cd was performed with the help of two low background NaI(Tl) crystals and enriched (to 68%) ^{106}Cd samples (≈154 g). New $T_{1/2}$ limits for the $\beta^+\beta^+$, β^+/EC and EC/EC decay of ^{106}Cd have been set in the range of $(0.3-4)\cdot10^{20}$ y at 90% C.L. [27].

3. NEMO collaboration experiment performed in the Frejus Underground Laboratory to study 2β decay of ^{100}Mo [28]. For background simulation the first version of the DECAY4 code [29] was used. The clear two neutrino 2β signal (1433 events during 6140 h) was observed, leading to a half-life $T_{1/2} = 0.95 \pm 0.04(\mathrm{stat}) \pm 0.09(\mathrm{syst})\cdot10^{19}$ y [28].

4. Heidelberg-Kiev collaboration: The background simulations were performed for the GENIUS project which aim is to increase the present sensitivity for 2β decay and dark matter search. Contributions from the cosmogenic activity produced in the Ge detectors and from their radioactive impurities as well as from contamination of the liquid nitrogen and other materials were calculated. External γ, μ and neutron backgrounds were considered also. The results of calculations evidently show feasibility of the GENIUS experiment [30].

In result, we can conclude:

1. The DECAY4 code is the powerful tool for simulation of the radionuclides decays in the wide range of decay's modes, emitting particles, etc.

2. The DECAY4 can be connected easily with the codes which simulate the particles propagation, like GEANT, EGS4, etc.

3. The code includes the most advanced databases: ENSDF, NuDat, EADL and others.

4. The event generator DECAY4 was used successfully in many underground experiments (Kiev, Roma-Kiev, DAMA-, NEMO-, GENIUS-collaborations).

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