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Code development for cumulative yield and decay heat using Geant4

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1. Introduction

In the early stage of development of Geant4 simulation, a lot of physicists and software engineers collaborated for the project participating in high energy physics experiments which were the original development purpose of Geant4. However, application field of Geant4 is growing and it has been used from the simulation of nuclear physics to space and medical physics. Thus additional physics models and functions are required for each application field.

Calculations related to the radioactive decay have been possible in Geant4 since version 2.0 [1]. This process is related to unstable nuclides and it seems to play a very important role in nuclear energy and nuclear safety. The simulation codes for the radioactive decay applications using Geant4 have been developed and validated through comparisons with the experimental and evaluated data considering the practical usage of Geant4.

2. Radioactive decay in Geant4

Radioactive decay is the process that unstable nuclei de-excite emitting particles and energies such as alpha particles, beta particles and so on. This process is important to low energy physicists and nuclear engineers. With this process, Geant4 could widen its application field to nuclear energy applications.

In order to work properly, it needs decay branching of each energy levels and information about consecutive gamma transition. Geant4 data library stores them separately. G4Radioactivedecay data files have the half-life, decay branch and q-value of each excitation level. On the other hand, G4PhtonEvaporation data files are related to excitation energies and their half-lives, angular momenta, internal conversion coefficients and gamma transitions. Both of them are originated from Evaluated Nuclear Structure Data File (ENSDF).

In this study, every physical process is omitted except for radioactive decay and particle transportation because simplified examples are easy to apply to wide uses rather than special cases.

3. Calculation of cumulative fission yield

Cumulative fission yield is the total number of atoms of that nuclide produced over all time after fission events [2]. The cumulative fission product distribution is very important for practical purposes such as waste storage, control of nuclear reactors, etc [3].

3.1 Definition of cumulative fission yield

It is very hard to define the cumulative fission yield for a radioactive nuclide. This is because some of nuclei decay to daughter nuclei while some produced from precursors. Thus more useful definition is used for cumulative fission yield as following: immediately at the end of an "infinite" irradiation at the rate of 1 fission per second or its rate of production if it is stable [2]. We calculated cumulative fission yield with this definition.

3.2 Input and output of the simulation code

As input, this code requires initial ratio of nuclei and their information such as charge of ion and excitation energy. As output, users can obtain atomic number and mass number distribution of fission products as well as cumulative fission yields of every isotopes including meta-stable states. Also, radiation spectra of electron, neutrino, gamma, etc. can be yielded with Root data format.

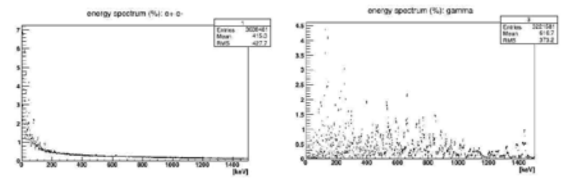

Fig. 1. Generated Root format files as the output of the code. The left is the electron energy spectrum and the right is that of gamma energy.

3.3 Validation of the simulation code (cumulative fission yield)

In order to check the result of the simulation code, we used fission yield data of ^{235}U.

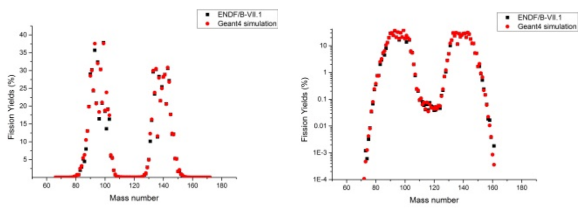

Fig. 2. The mass number distribution of cumulative yields of ENDF(black) and Geant4 simulation(red). The left is linear

scale and the right is log scale.

As input data, rates of fission products which produced from thermal neutron induced fission, e.g. independent fission yield of ^{235}U. This information is from ENDF/B-VII.1. Also, the results are compared with the cumulative fission product yield of ENDF/B-VII.1.

Fig. 2 shows that the result of Geant4 simulation is quite similar with the ENDF/B-VII.1 cumulative fission yields data.

Table I: Nuclides and yields (top 10 of abundance)

ENDF/B-VII.1		Geant4 simulation	
Nuclide	Yield	Nuclide	Yield
Xe134	0.078721	Xe134	0.07853
I134	0.078296	I134	0.078186
Te134	0.069725	Te134	0.069802
Ba138	0.067676	Ba138	0.068112
Cs138	0.067076	Cs138	0.068076
Xe133	0.066991	Cs133	0.067232
Cs133	0.066991	Xe133	0.067232
I133	0.066965	I133	0.0672
Cs135	0.06539	Mo95	0.065804
Ba135	0.06539	Zr95	0.065802

Most abundant 10 nuclides of ENDF/B-VII.1 are compared with the result of Geant4 simulation in table I. From Fig. 2 and Table I, we can recognize that the calculated fission yield is almost similar to cumulative fission yield of ENDF/B-VII.1 despite some conspicuous differences. However, these deviations are comes from not this code but Geant4 and developers are continuously solve these bugs.

4. Calculation of decay heat

Decay heat is the main source of nuclear energy. Moreover, it is closely related to nuclear safety. Therefore, prediction of decay heat of fission is very important.

4.1 Calculation of decay heat

The decay heat varies as a function of time because isotope composition in a reactor changes. Thus, we have to know the number of nuclide at time t. It can be obtained by solving a linear system of coupled first order differential equations that describe the buildup and decay of fission products [4]:

$$\frac{dN_i}{dt} = -(\lambda_i + \sigma_i \phi)N_i + \sum_j f_{j\to i}\lambda_j N_j + \sum_k \mu_{k\to i}\sigma_k \phi N_k + y_i F$$

Where N_i represents number of nuclides i, λ_i stands for the decay constant of nuclide i, σ_i is the average capture cross section of nuclide i, ϕ is the neutron flux, $f_{j\to i}$ is the branching ratio of the decay from nuclide j to i, $\mu_{k\to i}$ is the production rate of nuclide i per one neutron capture of nuclide k, y_i is the independent fission yield of nuclide i and F is the fission rate.

However, it is too complicated to solve the equation because about 1000 nuclides are produced by fission and we have to solve their simultaneous differential equation. Therefore, it is better to solve this problem with Monte Carlo method.

4.2 Input and output of the simulation code

The required data to calculate the decay heat of isotope is equal to that of cumulative fission yield, e.g. initial ratio of nuclei and their information. As output, this code shows that multiplication of time and each type of radiation such as alpha, beta, gamma and emitted energy by neutrino. Furthermore, total decay heat which is the sum of above except emitted energy trough neutrino is reported.

4.3 Validation of simulation code (decay heat)

In order to validate the result of decay heat simulation, we compared the result with the decay heat experimental data performed at Oak Ridge National Laboratory (ORNL). We used independent fission product yield of ^{235}U in ENDF/B-VII.1 as input data

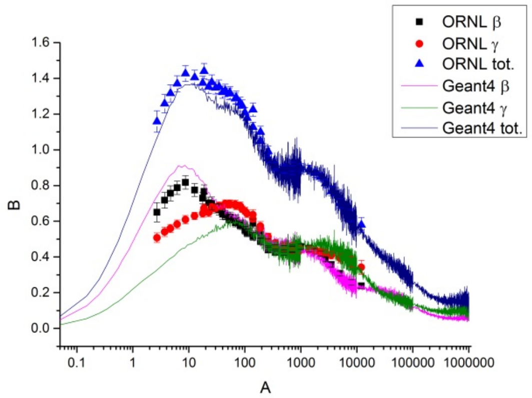

Fig. 3. The curves are calculation result of Geant4 code and data points are from ORNL experimental data.

Calculated beta decay energy and gamma decay energy show differences with experimental data. As a result, the total decay heat is somewhat less than the references although differences are compensated.

5. Conclusions

Geant4 simulation developers and users have tried to widen its application fields. With the present version of Geant4 we can make useful simulation code for nuclear energy application. Moreover, as the demand is rising, more physical models and processes are being added.

Although it is not easy to make simulation code with Geant4 compared with other simulation tools, it has more potential. Furthermore, providing the newest data and improved process by patch and update, we can obtain reliable result from the Geant4.

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