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Calculation of the isotope composition and induced activity in irradiated materials of innovative accelerator-driven systems

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Abstract

The paper describes the SNT.1 system for calculating the isotopic composition and induced activity of irradiated materials in innovative accelerator-driven systems (ADS). The SNT.1 algorithm, a list and the format of input data, a list of the evaluated nuclear data libraries to be used in calculations, and the potential calculation options are presented. The activity calculation for the water cooling of the Ta target in the TRADE project is presented, and the calculation results are compared with those obtained using other codes. The concentration and the activity of the nuclides formed during irradiation of a lead-bismuth target have been calculated with due regard for the variations in the accelerator current during irradiation. The possibility for neural networks to be used for the approximation and restoration of data, such as the reaction cross-sections, has been studied. The RBF and GRNN neural network structures were selected to approximate data on the ^{209}Bi (n, 3n) ^{207}Bi and ^{54}Fe (n, p) ^{54}Mn reaction cross-sections. Neural networks were used to restore data for the total cross-section of reactions of interaction with ^{209}Bi nuclei. The approximation quality was assessed using agreement factors.

Keywords: Transmutation; Activity calculation; Irradiated materials; Nuclear data; Reaction cross-sections; Neural networks.

Transmutation of nuclear waste

Transmutation of long-lived nuclei from spent reactor fuel into stable or short-lived nuclides is looked upon as an alternative to waste disposal and is expected to lead to greatly reduced nuclear plant impacts on the environment. Thanks to transmutation of waste, it is possible to achieve a radiologically cleaner nuclear power. Therefore, it becomes essential to develop codes for calculating the isotope composition and the induced activity of irradiated materials. Such calculations are important both for the theoretical and practical aspects of the nuclear power plant operations, as well as for the fields of medicine and ecology.

Most of the danger comes from long-lived transuranic elements. Time-variable values of the relative radiotoxicity of long-lived transuranic elements are presented in Table 1 (radiotoxicity of plutonium for 10 years was taken as unity).

Over time, the activity of spent nuclear fuel (SNF) comes down thanks to the decay of short-lived fission products, still major contributors to the activity for hundreds of thousands of years have been long-lived transuranic elements and fission products.

The key strategies in solving the radioactive waste problem are the following [1–3]:

- direct disposal of RW (current strategy);
- partial reduction in the amounts of Pu, minor actinides and fission products through transmutation with further geological disposal;
- reduction in the amounts of nuclear waste, to such extent as possible, through transmutation into stable isotopes, e.g. using accelerator-driven systems (ADS).

This requires emphasis to be placed on the development and use of nuclear plants with an external neutron source that can be also used for generation of isotopes for medical applications.

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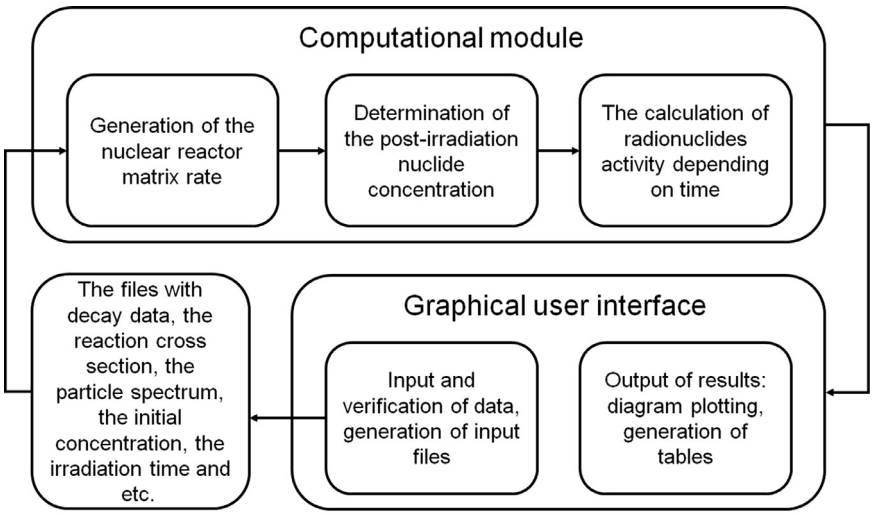

Fig. 1. SNT.1 operation flowchart.

Table 1
Time-variable values of the relative radiotoxicity of long-lived transuranic elements.

Nuclide	$T_{1/2}$, years	Storage time, years			
		10	100	1000	10,000
^{238}Pu	87.7	233	110	0.3	1.5
^{239}Pu	$2.4{\cdot}10^4$	1	1	0.97	0.75
^{240}Pu	$5.56{\cdot}10^3$	3.6	3.6	3.3	1.3
^{241}Pu	14.4	45	56	13	0.02
^{242}Pu	$3.7{\cdot}10^5$	0.05	0.05	0.05	0.05
^{237}Np	$2.1{\cdot}10^6$	0.02	0.02	0.02	0.02
^{241}Am	432	63	54	13	0.02
^{243}Am	737	3.3	3.3	3.1	1.8
^{244}Cm	18.1	600	20	3.3	1.3

At the present time, different organizations worldwide carry out investigations in the field of separation and transmutation technologies.

Calculations and studies in the field of transmutation and activation of materials, ADS and nuclear medicine use advanced software and codes making it possible to calculate different ADS characteristics, isotope compositions, activities of materials, irradiation doses, and radiation damage.

Interactive system for calculation of the isotope composition and activity in irradiated materials

Calculations of the isotope compositions and induced activities in materials are based on solving the system of Bateman's equations realized by a number of methods: numerical solution, solution by matrix exponent method and analytical solution (Bateman's formula).

The equation for the concentration of an individual k^{th} nuclide looks as

$$\frac{dN_i(t)}{dt} = \sum_{k\neq i} (\lambda_{ik}^r + \lambda_{ik}^d) \cdot N_k(t) - (\lambda_i^r + \lambda_i^d) \cdot N_i(t),$$

where $N_i(t)$ is the concentration of the ith nuclide at the time t; λ_{ik}^r and λ_{ik}^d are the rates of the nuclear reaction and the radioactive decay as the result of which the kth nuclide transforms into the ith nuclide; λ_i^r is the rate of the ith nuclide transmutation in nuclear reactions, and λ_i^d is the rate of the radioactive decay of such nuclide.

To solve the system of Bateman's equations, the SNT.1 software package [4] was used, in which the concentration of isotopes is calculated by matrix exponent method. In this case, the solution is sought in the form

$$N(t) = \exp(tC)N(0).$$

By setting $tC = A$, we shall expand the exponent in a Taylor series. Then the solution will have the form

$$\exp(A)N(0) = \left(1 + A + A^2/2! + A^3/3! + \ldots\right)N(0).$$

The SNT.1 package is a computational model and a user graphic interface. Computational model is a set of Fortran-based programs. The user input/output interface is written in the C# language using the Microsoft Visual Studio.Net 2008 development environment. Such combination provides for a great amount of computations, on the one hand, while, on the other hand, for a simple and understandable input of needed data and output of results in a convenient form, that is, as diagrams and tables that can be stored, reformatted and opened through different applications (Word, Excel, MathCad and others). The package operation flowchart is shown in Fig. 1, and the interface is shown in Fig. 2.

The nuclide concentration and activity are calculated in the process of irradiation and when the irradiated material is cooled. The input data represent spectra of particles, cross-sections of nuclear reactions in the considered range of energies, and data on the radioactive decay of the nuclei under investigation. All these calculations are performed with regard for the irradiation conditions (options with a variable accelerator current and with a variable spectrum). The option with a time-variable accelerator current requires presetting the current values and the time intervals for which they were maintained. Spectra and time