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Interactive information system for simulation and visualization of nuclear transformations–Nuclear evolution software

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Abstract

The present paper gives a brief review of the methodology for modeling evolutions of fuel isotopic composition by the set of ordinary differential equations describing nuclide transmutation. Algorithms for modeling and calculation of main parameters of nuclear transformations based on directed graphs are suggested, which improves the speed and accuracy of calculations. Description is given of the designed software system for modeling radioactive decay transformations and transformations caused by particle fluxes (neutrons, protons, etc.). Specific features and functionality of this system are defined.

Distinguishing features of the system include simplicity, developed user-friendly interface, high degree of automation of all stages of user work, simulated process imaging and convenient tools for calculation management and processing of results. The described system is intended for wide range of users from students and post-graduates to university professors and researchers, and can be used as the instrument in scientific research and in education. The presented system is a convenient tool for assessment of concentration of any isotope in the decay chain depending on the integral flux and time with varying starting quantities of isotopes.

Advanced licensed software tools and libraries of visual reference components from leading global producers were utilized in the development of the system along with author's own developments, which allowed developing user-friendly interface and keeping abreast with leading software developments. Results of modeling are displayed in the form of interactive tables and characteristic curves. Examples are given of the use of the suggested software tools.

Keywords: Radioactive waste; Transmutation; Decay chain; Graph theory; Bateman equations; Information systems; Interactive interface.

Introduction

Control of conditions and evolution of isotopic composition of nuclear fuel is the important aspect of nuclear power generation. Modeling the processes of nuclear transformations has applications within the wide range of applied and theoretical studies associated with development of nuclear technologies. In particular, it is necessary as of the present moment to solve problems related to the utilization of irradiated nuclear fuel. One of the main methods suggested for reprocessing spent reactor fuel is based on the transmutation of hazardous fission products accumulated in the fuel after its irradiation in fission reactors or in the reactor systems with subcritical cores where nuclear transformations are also determined by nuclear reactions [1]. Therefore development of dedicated computer codes for modeling transmutation of nuclides becomes important.

The system gives the possibility to automatically construct and on-line display on the screen the chain of nuclide transformations taking place in the process of radioactive decay and, also, as the result of reactions induced by neutrons, to estimate the number of nuclei of the target nuclide under irradiation and during cooling down of the target.

Interactive reference and information system is integrated in the system containing the required information about characteristics of the most part of known nuclides of 112 chemical elements. Possibility of switching to remote data bases for obtaining the properties of exotic nuclides is also implemented.

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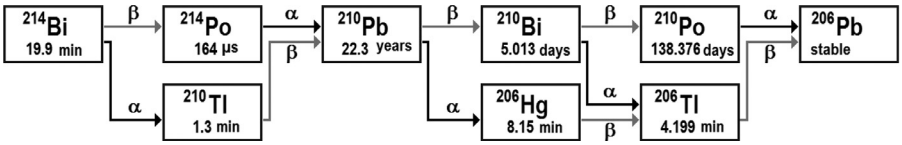

Fig. 1. ^{214}Bi decay chain.

Specific features of modeling and calculation of main characteristics of the processes

For decay chains when radioactive substance X_1 is transformed into X_2, X_2 is transformed into X_3 and so on, the balance of quantities of nuclides is determined by the usual decay conditions. Rate of transformation of X_k into X_{k+1} is proportional to λ_k, while rate of transformation of X_{k-1} into X_k is proportional to λ_{k-1}. Variation of concentrations of isotopes with time is described by the set of n ordinary differential equations (ODE) as follows:

$$\begin{aligned} dN_1(t)/dt &= -\lambda_1 N_1(t); \\ dN_2(t)/dt &= -\lambda_2 N_2(t) + \lambda_1 N_1(t); \\ dN_n(t)/dt &= -\lambda_n N_n(t) + \lambda_{n-1} N_{n-1}(t). \end{aligned} \quad (1)$$

Calculation of sets of differential equations describing decays in radioactive decay chains results in significant expenditures of CPU time even when advanced computers and standard numerical methods are used. This is explained by the fact that in numerical integration of the set of equations the value of the integration step cannot exceed according to the most rough estimations the half-life of the most short-lived isotope in the decay chain. The case when isotopes whose half-lives differ by several orders of magnitude are present in the same decay chain appears to represent a complex and time-consuming problem.

In the simplest case when at the initial moment there are no daughter nuclei and the number of parent nuclei is equal to N_{10} solution of each k-th equation has the following form [2]:

$$N_k(t) = N_{10} \sum_{i=1}^{k} C_i e^{-\lambda_i t}, \quad N_{10} = N_1(0), \quad (2)$$

where C_i is the factor in the Bateman solution calculated according to the following formula:

$$C_i = \prod_{i=1}^{k-1} \lambda_i \Big/ \sum_{i=1}^{k} (\lambda_j - \lambda_i), \quad j \neq i. \quad (3)$$

Calculation of concentration of nuclei in the case of "branching" of the decay chain. Two or more competing processes of nuclear transformations take place for a number of nuclides. Assumption was made that branching events within the scheme of nuclide transformation occur in the process of transmutation independently from each other. It is reasonable to represent decay chains containing branching in the calculations of activity in these chains in the form of several independent linear chains and following this to perform calculation of transmutation parameters using formulas (2) and (3) [3].

For example, six conventionally independent unique paths resulting in the formation of ^{206}Pb from ^{214}Bi exist in the ^{214}Bi decay chain presented in Fig. 1:

^{214}Bi→^{214}Po→^{210}Pb→^{210}Bi→^{210}Po→^{206}Pb;
^{214}Bi→^{210}Tl→^{210}Pb→^{210}Bi→^{210}Po→^{206}Pb;
^{214}Bi→^{214}Po→^{210}Pb→^{210}Bi→^{206}Tl→^{206}Pb;
^{214}Bi→^{210}Tl→^{210}Pb→^{210}Bi→^{206}Tl→^{206}Pb;
^{214}Bi→^{214}Po→^{210}Pb→^{206}Hg→^{206}Tl→^{206}Pb;
^{214}Bi→^{210}Tl→^{210}Pb→^{206}Hg→^{206}Tl→^{206}Pb.

Then, under the assumptions made above, number $N_k(t)$ of nuclei of nuclide k at a certain moment t can be obtained as the sum of the number of nuclei of this nuclide calculated according to all linear chains n from the starting nuclide to nuclide k:

$$N_k(t, N_0) = \sum_n \left(N_{10} \prod_{i=1}^{k-1} q_i \sum_{i=0}^{k} C_i e^{-\lambda_i} \right), \quad (4)$$

where q_i is the fraction of decay, and C_i is calculated according to formula (3)

For reactions induced by particles (neutrons, protons, etc.) reaction rate depends on the properties of nuclei of the nuclide and the spectrum of these particles. Probability of nuclear decay per unit time under the flux of particles of different types or under irradiation (for the sake of convenience this value is denominated in the present paper as Λ similarly to decay constant λ and is called the nuclide decay constant under particle flux) is described by the following equation:

$$\Lambda_i = \lambda_i + \sum_f \sigma_{if} \Phi_f, \quad (5)$$

where λ_i is the decay constant characterizing the rate of natural radioactive decay of nuclide i; Φ_f is the particle flux density f; σ_{if} is the micro-section of reactions (f, γ), (f, α), (f, β), (f, 2n), (f, 3n) … of interaction of particles f with nuclei of the nuclide resulting in its transformation into other nuclide. Value (σ_{if} Φ_f) characterizes the rate of transmutation of i-th nucleus of the nuclide under the effects of flux of particles f. Inverse value (σ_{if} Φ_f)$^{-1}$ is the average lifetime of the nuclide under the flux of particles [4,5].

In the case in question Λ_i must be taken into account in the solution of the set of equations (1) instead of decay constant λ_i.

Specific activity Q of radionuclide in the target in the calculation per one gram of starting chemical element is equal to:

$$Q_i(t) = \lambda_i \cdot N_A \cdot C \cdot N_i(t)/M, \quad (6)$$

where N_A is the Avogadro number; C is the isotopic concentration of the main starting nuclide; $N_i(t)$ is the number of