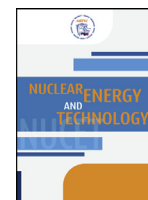


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Interactive information system for simulation and visualization of nuclear transformations—Nuclear evolution software

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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.

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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.

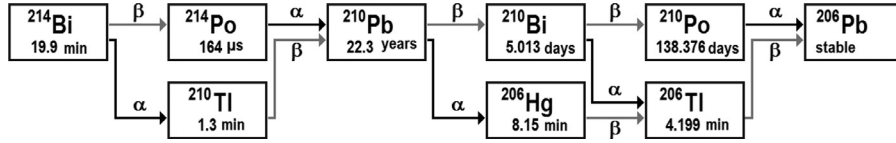
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Fig. 1. ^{214}Bi decay chain.

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]:

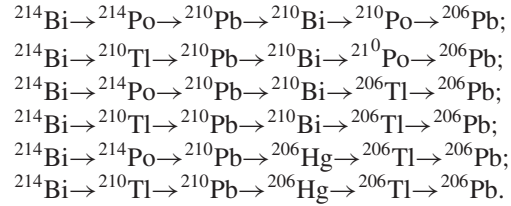
$$N_k(t) = N_{10} \sum_{i=1}^k C_i e^{-\lambda_i t}, \quad N_{10} = N_1(0), \quad (2)$$

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

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

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:



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 $(\sigma_{if} \Phi_f)$ characterizes the rate of transmutation of i -th nucleus of the nuclide under the effects of flux of particles f . Inverse value $(\sigma_{if} \Phi_f)^{-1}$ 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

nuclei of i -th radionuclide at time moment t ; M is the average atomic mass of the starting chemical element. Possibility to calculate specific activity of accompanying radionuclides allows performing analysis of the process of obtaining the radionuclide and selecting optimal parameters of the irradiation and cooling down regimes [3].

In the software package under discussion the chain of transformations is represented in the form of directed graph nodes of which are the isotopes or nuclides constituting the decay chain and the edges correspond to the mutual transformations of nuclides in the process of transmutation. Direction of the edges corresponds to the direction of transformation of nuclides, i.e. from the parent nuclide to the daughter nuclide. This allows treating the chain of nuclear transformations as the mathematical object with application in the operations performed with it of special approaches and methods typical for operations with graphs.

The following three types of nodes can be defined for the graph of nuclear transformations:

- Zero generation node, i.e. node into which neither of the edges enters. Zero generation nodes correspond to isotopes preset at the initial time moment.
- Last generation node, i.e. node from which neither of the edges exits. Such nodes represent stable isotopes or isotopes for which the system failed to find the data needed for modeling.
- Target node, i.e. node parameters of which must be calculated.

The highest chances to get into the uninvestigated area for the problem of nuclide transmutation are to examine possible candidates for the role of daughter isotopes for obtaining the target nuclide as a fission fragment. Within this layout search for subsequent isotopes is performed at each successive step on the basis of preceding steps. The process is continued until the system finds a stable isotope or element for which there are no input data available.

For correct definition of the vector of unknowns of the set of transmutation ordinary differential equations it is necessary to construct all possible unique linear chains of nuclear transformations realized under irradiation of isotopes. It is intended to use for this purpose the algorithms used in the search for paths in the maps of unknown terrains.

Depth First Search method (DFS) was applied for determining the path of formation and singling out linear chains. Search algorithm is described in the following way: it is necessary to find for each untraveled node all the adjacent untraveled nodes and repeat the search for them. Progressive processing of all nodes of the graph which can be reached from the preset node S where the search starts is made by the method of systematic traveling (visiting) the nodes of the graph, when movements from the current node are made ahead along the edge (to not yet processed node) in all cases when possible and return movements are made from the current node backwards along the traveled edge (to the previously

traveled node) if movement ahead from the current node is not possible [6].

Description of the system and its functionality

The NES (Nuclear Evolution Software) system is the software product representing independent application with direct access to the remote or local databases. The system possesses wide range of navigation tools intended to help the user in determining the nuclei and the data of interest. Area for plotting decay chains and area for plotting the graphs of concentrations of nuclei are available in the main NES window. The system also presents the values of concentrations of activity and toxicity in certain time points according to the user's choice. Significant attention was paid in the process of system development to the main principles of development of interactive interfaces [7].

The structure in the form of directed graph elements of which are represented by isotopes is displayed by the system in the main window (Fig. 2). In each element the system displays the name of the isotope and its half-life; each element is highlighted according to its own color code. Probability of decay according to a certain decay path is illustrated by the color of the arrow. The higher is the probability, the brighter is the arrow representing the type of decay in question. Graphs of time dependences of isotopes concentrations are plotted below in a separate window. Possibility to obtain numerical values for the preset time points is also implemented. Isotopic composition is preset in the upper left corner of the screen in the form of the isotope name and its concentration.

Reference system “Nuclide Explorer” (Provodnik nuklidov)—the built-in presentation subroutine intended for simplification of access to reference data—was realized in order to facilitate data input.

The reference and information system in question covers the combination of properties for more than 3500 isotopes of 112 chemical elements. Besides the data on the composition of nuclei, the database also contains reference data on the main properties of isotopes of chemical elements, such as mass, excess mass, type of decay, half-life, abundance of the nuclide in natural mixture of isotopes (%), spin and parity of the ground state. The above values are accompanied with values of standard uncertainties. Evaluated values of half-lives are presented for radioactive nuclides. “Stable” is indicated for stable nuclides instead of the half-life value. The data were obtained on the basis of information contained in the databases of the Nuclear Data Center of the Japan Atomic Energy Agency [8] and the Brookhaven National Nuclear Data Center (NNDC) [9]. Data on micro-sections of reactions induced by thermal neutrons were prepared on the basis of the data in the FENDL-2.1 library (Fusion Evaluated Nuclear Data Library) [10]. Access to the data is provided through the diagram of nuclides or through the periodic system.

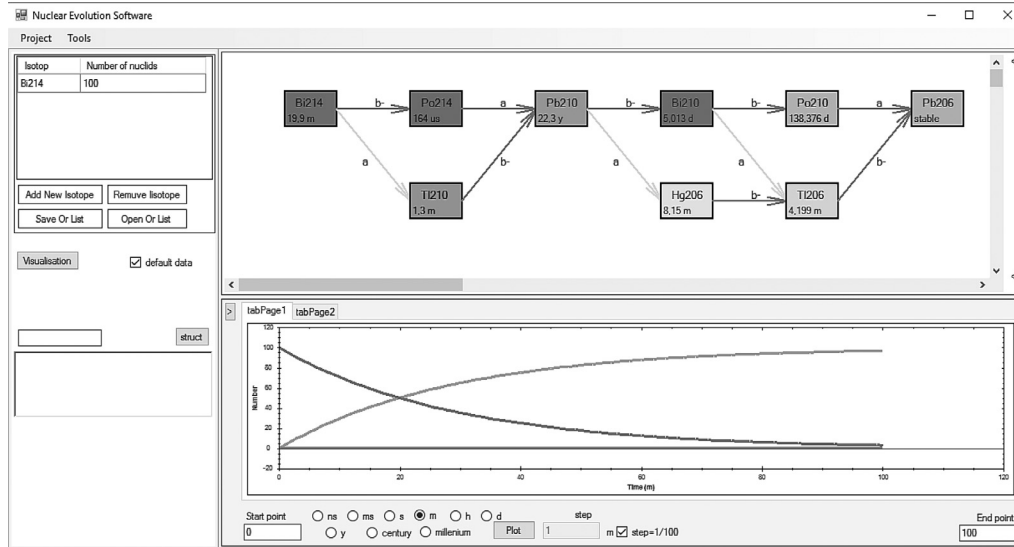


Fig. 2. Appearance of the main NES window.

Modeling evolution of isotopic composition of spent VVER-1000 nuclear fuel after long-term cooling

Modeling of long-term cooling of spent VVER-1000 nuclear reactor fuel was performed in order to demonstrate the potential of the system. Spontaneous processes of fission and radioactive decay continue after unloading the spent nuclear fuel (SNF) from the reactor core with short-lived radionuclides disappearing and new nuclides born. SNF remains to be a powerful source of α -, β -, γ - and neutron radiation and heat release during extended periods of time. Fragment of the modeling result for the decay chains in the spent VVER-1000 nuclear reactor fuel is presented in Fig. 3. Elements constituting the initial isotopic composition of SNF are indicated in the boxes [5,11].

Graphic version of calculation of isotopic composition evolution in the SNF after extended cooling period is presented in Fig. 4. Considering the radio-ecological characteristics of the SNF and the results of modeling, it can be characterized, first of all, as highly radioactive material which, from the environmental viewpoint, represents hazard not only in short-term, but in long-term perspective as well.

Conclusions

Main methods for calculation of evolution of nuclear fuel isotopic composition were examined. Algorithm of calculation of main parameters of transmutation based on directed graph of nuclear transformations was developed on the basis of solution of sets of ordinary differential equations suggested by Bateman.

Interactive system was developed giving the user the possibility to perform evaluation of efficiency of nuclide transmutation in the process of SNF cooling under different conditions. CPU time needed for calculations was significantly reduced

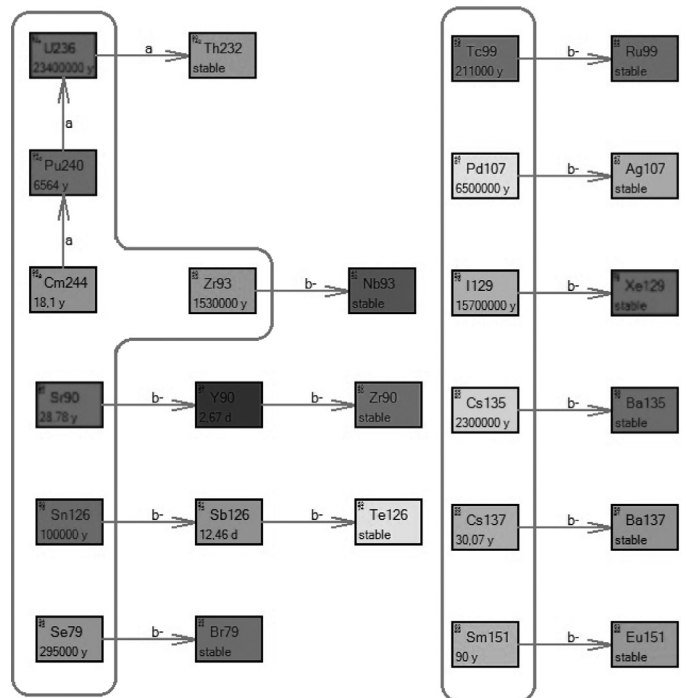


Fig. 3. Fragment of decay chain modeled by the system for spent VVER-1000 nuclear reactor fuel.

due to the implemented code optimization. The software system in question was applied for transmutation modeling described in Ref. [12].

In contrast to numerous scientific software complexes in which different phases of work are performed by the users in different, sometimes even “non-uniform” applications with different interfaces and with different inherent logic of interactions between the objects, the NES was developed in the form of integrated environment combining all user software

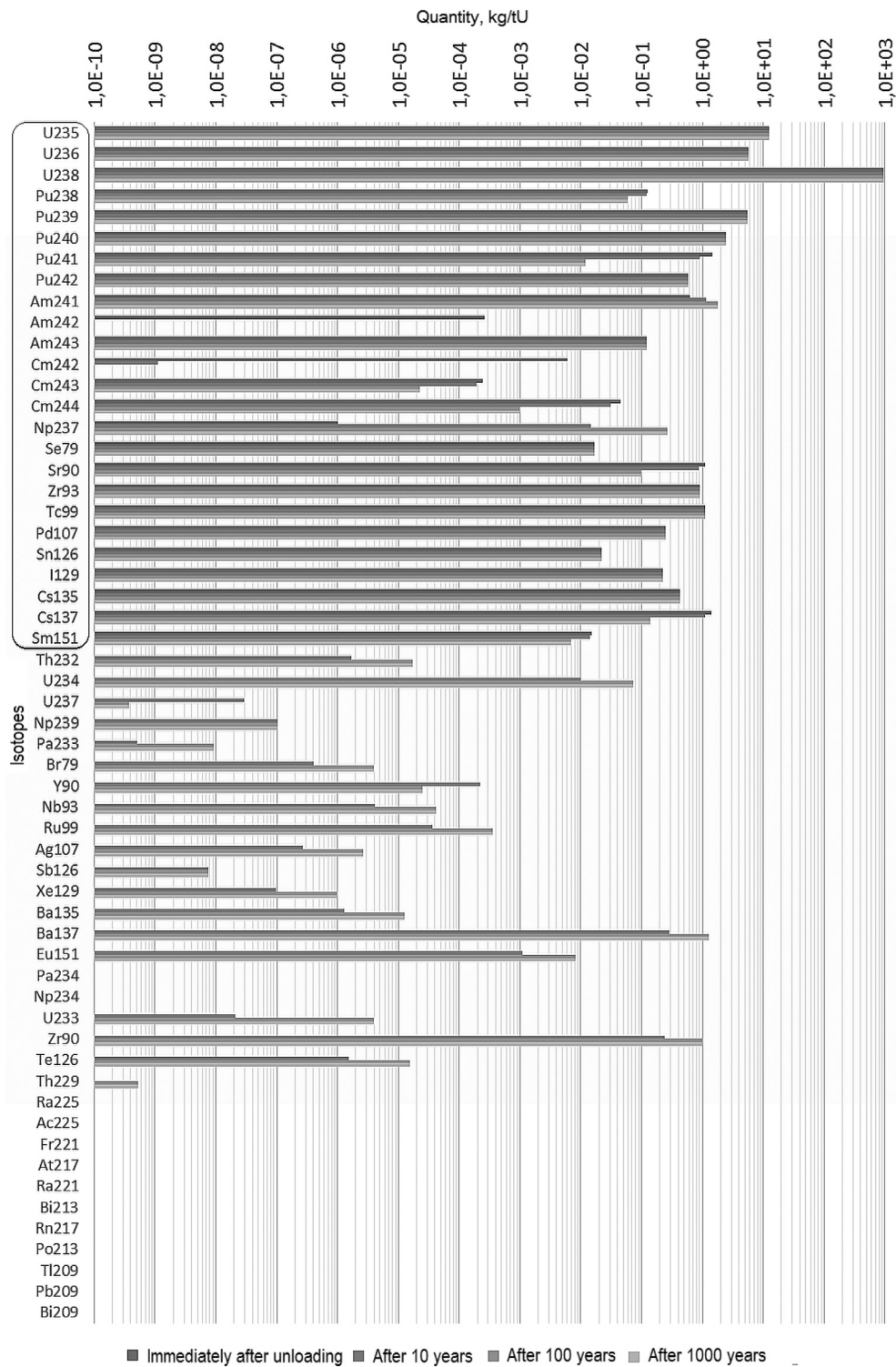


Fig. 4. Evolution of isotopic composition in the VVER-1000 reactor spent nuclear fuel.

tools into the unified application with unified interface and common logic of objects functioning.

All phases of user work including preparation and editing the input data, automated analysis and processing of results are represented visually which provides for the ease of use, quick perception of the results and high level of informativity.

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