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METHOD OF ESTIMATING THE SENSITIVITY OF A CALCULATED NUCLIDE VECTOR TO DEVIATIONS IN INITIAL DATA

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Abstract

The application of perturbation theory algorithms in modelling of nuclides transmutation is considered. The perturbation theory is used to construct the analytical technique of sensitivity analysis. It is shown that such algorithms have to be used in modelling of lifetime performance of nuclear power installations with the Monte Carlo method. The present approach differs from others by consistent use of analytical methods.

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INTRODUCTION

The overall world trend in research in the nuclear engineering field is to be seen as an increase in the proportion of detailed-theoretical modelling of the characteristics of nuclear systems. In order to satisfy the increasing requirements for accuracy in the theoretical prediction of the characteristics of nuclear reactors and nuclear systems of different types, mathematical methods, algorithms and programs are being developed which make it possible to model comprehensively a particular system as a complex object, to take into account the effect of uncertainty of the initial data and approximations of theoretical models, and to perform a detailed analysis of various physical processes with allowance for their actual interaction, technical conditions and limitations.

The packages of programs created to solve a problem in this field are universal at the algorithm level and their structure enables them to be adjusted to the type of system in question through selection of corresponding program units modelling a specific physical process (preparation of initial data, calculation of fields of radiation, temperatures, nuclides, etc.). One of the problems of organising a complex calculation is that of co-ordinating the information flows (initial data for some modules and results of calculations for others). Here it is important to evaluate the quality of the results obtained by particular program modules from the point of view of using them in joint modelling. This calls for estimation of the error introduced by the initial data in the program modules involved in the complex calculation and estimating the accuracy requirements for such modules.

New conceptions of the application of nuclear engineering including different ways of managing radioactive waste, transmutation of long-lived radioactive fission products and minor actinides call for prediction of the long-term consequences with different scenarios for the development of power engineering. Systems analysis in this area involves estimating the effect of uncertainty of nuclear data and the models employed on the results of calculating the status of the whole system. This is particularly relevant for estimating the prospects of using accelerator-controlled nuclear systems for eliminating long-lived toxic waste from nuclear power plants [5]. For this it is necessary to determine the requirements with respect to initial nuclear data and theoretical models on the basis of the systems analysis requirements.

It should also be noted that in many problems, where the accumulation or elimination of nuclides in nuclear reactors is modelled, the Monte Carlo method is used to calculate neutron and

photon fields owing to the complex structure of the zones under irradiation [6]. The inevitable statistical error determines the basic limit for refining nuclear data.[1]

In this paper the author presents a tool for determining the requirements for refining constants and programs in nuclear power systems analysis problems. Generally, the estimation of the sensitivity of the results of calculation to the nuclear data can be carried out in numerous direct ways. However, if it is a question of statistical methods of calculation or a randomly distributed initial value, the only method of estimating the error is to use a model of linear error propagation, employing the method of small perturbations [2].

Therefore, an algorithm of the method of perturbations and a corresponding computer program have been developed for modelling the nuclide composition of materials of a nuclear system with the Monte Carlo method and for estimating the effect of statistical uncertainty of nuclear data.

This paper is devoted to developing a mathematical model, methods, algorithm and programs for calculating the evolution of fields of nuclide concentrations and estimating the sensitivity of the result to deviations of the nuclear data, including those bearing a random character.

The evolution of the field of nuclide concentrations in materials of the system in question is described by a dynamic model in lumped parameters. The coefficients of the matrix of the nuclide transmutations are determined from calculation of the steady-state neutron and photon fields and are normalised taking into account the complete capacity of the plant. Here it is assumed that variations in the parameters of the system are small and that a small enough time interval can be selected for the spectral characteristics within it to be considered constant. The stability of the solution of the system of equations is achieved through the use of an analytical algorithm.

MATHEMATICAL MODEL AND APPROXIMATIONS EMPLOYED

The evolution of the field of nuclide concentrations in the materials of a nuclear reactor or system is described by a dynamic model in lumped parameters [3]. Time is considered here as an independent variable.

$$\frac{d\vec{r}}{dt} = \hat{B} \cdot \vec{r} + \hat{A} \cdot \Phi \cdot \vec{r} \,, \tag{1}$$

where $\vec{r}(t) = \left[r_1(t), r_2(t), \ldots r_N(t) \right]^T$ is the column vector of the nuclide concentrations; $\hat{B}$ is the square matrix of the nuclide transmutation as a result of radioactive decay; $\hat{A}$ is the square matrix of transmutations as a result of neutron reactions; Φ is the integrated neutron flux.

The system of equations may be written in the form of a system of equations for the segregated chains of transmutations which are represented by the usual differential equations

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[1] It is clear that refinement of nuclear data which results in a considerably smaller error than the minimum statistical error is hardly worthwhile.

$$\begin{cases} \dfrac{dN_0(t)}{dt} = -a_0 \cdot N_0(t) + q_0 \\ \dfrac{dN_1(t)}{dt} = -a_1 \cdot N_1(t) + l_0 \cdot N_0(t) \\ \dots \\ \dfrac{dN_k(t)}{dt} = -a_k \cdot N_k(t) + l_{k-1} \cdot N_{k-1}(t), \end{cases}$$

(2)

where q_0 is the source of the initial nuclide of the chain; N_0 is the concentration of the initial isotope; N_k is the isotope which is determined in the chain; α_i is the probability of disappearance of the i-th nuclide; λ_l is the coefficient of transmutation of the i-th nuclide to the $(i+l)^{th}$.

The complete solution is presented in the form of the sum.

$$N_m(t) = \sum_{ic} n_{ic}(t), \tag{3}$$

where $N_m(t)$ is the concentration of the m-th nuclide; $n_{ic}(t)$ is the solution along the ic^{th} chain.

The solution for the segregated chain is represented as:

$$n_k(t) = n_0(0) \cdot \prod_{i=0}^{k-1} l_i \cdot \sum_{j=0}^{k} \frac{\exp(-a_j \cdot t)}{\prod_{i \neq j} (a_i - a_j)} + q_o \prod_{i=0}^{k-1} l_i \left[\frac{1}{\prod_{j=0}^{k} a_j} - \sum_{j=0}^{k} \frac{\exp(-a_j \cdot t)}{a_j \cdot \prod_{i \neq j} (a_i - a_j)} \right]. \tag{4}$$

Not all coefficients of nuclide transmutations are estimated with the same accuracy. By analysing the sensitivity of the results to variations in the initial data, it is possible to estimate the permissible error with which the rates of processes on individual nuclides ought to be estimated. It is convenient to introduce into the consideration a pseudo-nuclide, the concentration of which is proportional to the energy released in the course of irradiation or to some other functional that can be calculated in similar fashion. This nuclide is determined for those material zones where the power conservation condition has to be fulfilled. It is not difficult to generalise such an approach to any model of the conserved value, i.e. to introduce certain weighting coefficients for the material zones, which determine the contribution to the general conserved functional. The proposed algorithms are applicable for the most general statement of the problem without significant limitations as to the type of nuclear system modelled [4].

The deviation in concentrations is presented in the form

$$dN_m(t) = \sum_{ic} dn_{ic}(t). \tag{5}$$

If the calculations are performed over finite time intervals, the solution for each of them is the result of the action of the linear operator on the nuclide vector:

$$r_j(t) = u_{ij}(t) \cdot r_i(0). \tag{6}$$

The variation for each isotope

$$dr_l(T) = \sum_i r_i(0) \cdot \frac{\partial u_{il}(T)}{\partial a_{km}} \cdot da_{km}, \tag{7}$$

where $\frac{\partial u_{il}(T)}{\partial a_{km}}$ is the derivative of $u_{il}(t)$ with respect to the parameter α_{km};, da_{km} is the variation of the parameter of k-th nuclide incineration for the m-th process ($da_{km} = ds_{km} \cdot \Phi$).

In the event of small deviations we have:

$$\frac{dr_l(T)}{ds_{km}} = \sum_i r_i(0) \cdot \frac{\partial u_{il}(T)}{\partial s_{km}}, \tag{8}$$

where σ_{km} is the cross-section of the m-th process on the k-th nuclide.

It is necessary to estimate the contributions for each chain:

$$\frac{d_{t,ic} r_l(T)}{ds_{km}} = r_i(0) \cdot \frac{\partial u_{il}^{ic}(T)}{\partial s_{km}}. \tag{9}$$

All variations in the linear model may be represented as:

$$dh_{ik}(t) = \sum_k \frac{\partial h_{ic}(t)}{\partial a_k} \cdot \frac{\partial a_k}{\partial s_c^l} + \sum_k \frac{\partial h_{ic}(t)}{\partial l_k} \cdot \frac{\partial l_k}{\partial s_c^l}. \tag{10}$$

The formula for estimating the derivative with respect to the nuclide elimination parameter:

$$\frac{\partial n_k(t)}{\partial a_m} = n_0(0) \cdot \prod_{i=0}^{k-1} l_i \cdot \left[\sum_{j \neq m} \left(\frac{\exp(-a_m \cdot t)}{(a_j - a_m) \cdot \prod_{i \neq m} (a_i - a_m)} + \frac{\exp(-a_j \cdot t)}{(a_j - a_m) \cdot \prod_{i \neq j} (a_i - a_j)} \right) \right]$$

$$- n_0(0) \cdot \prod_{i=0}^{k-1} l_i \cdot \left[\frac{t \cdot \exp(-a_j \cdot t)}{\prod_{j \neq m} (a_j - a_m)} \right] - q_o \cdot \prod_{i=0}^{k-1} l_i \cdot \left[\frac{1}{a_m \prod_{j=0}^{k} a_j} + \left(\frac{t}{a_m} - \frac{1}{a_m^2} \right) \cdot \frac{\exp(-a_m \cdot t)}{\prod_{j \neq m} (a_j - a_m)} \right], \tag{11}$$

$$+ q_o \cdot \prod_{i=0}^{k-1} l_i \cdot \left[\sum_{j \neq m} \left(\frac{\exp(-a_m \cdot t)}{a_m \cdot (a_j - a_m) \cdot \prod_{i \neq m} (a_i - a_m)} + \frac{\exp(-a_j \cdot t)}{a_j \cdot (a_j - a_m) \cdot \prod_{i \neq j} (a_i - a_j)} \right) \right].$$

The derivative with respect to the parameter for transmutation of nuclide to nuclide

$$\frac{\partial n_k(t)}{\partial \lambda_l} = n_0(0)\cdot\prod_{i\neq m}^{k-1}\lambda_i\cdot\sum_{j=0}^{k}\frac{\exp(-a_j\cdot t)}{\prod_{i\neq j}(a_i-a_j)} + q_o\cdot\prod_{i\neq m}^{k-1}\lambda_i\cdot\left[\frac{1}{\prod_{j=0}^{k}a_j}-\sum_{j=0}^{k}\frac{\exp(-a_j\cdot t)}{a_j\cdot\prod_{i\neq j}(a_i-a_j)}\right]. \quad 12)$$

The derivative with respect to the initial nuclide concentration

$$\frac{\partial n_k(t)}{\partial n_0(0)} = \prod_{i=0}^{k-1}\lambda_i\cdot\sum_{j=0}^{k}\frac{\exp(-a_j\cdot t)}{\prod_{i\neq j}(a_i-a_j)} + q_o\cdot \quad (13)$$

The derivative with respect to the magnitude of the nuclide source

$$\frac{\partial n_k(t)}{\partial q_0} = \prod_{i=0}^{k-1}\lambda_i\cdot\left[\frac{1}{\prod_{j=0}^{k}a_j}-\sum_{j=0}^{k}\frac{\exp(-a_j\cdot t)}{a_j\cdot\prod_{i\neq j}(a_i-a_j)}\right]. \quad (14)$$

Modelling in a medium with randomly varying characteristics may be performed in the form of a branching process [1] represented by the Markoff process as:

$$\boldsymbol{m}(t)=(m_1(t),m_2(t),m_3(t),\ldots m_n(t)) \; . \quad (15)$$

The probability for the i-th nuclide is:

$$P(i\rightarrow i) = 1-h\cdot\sum_k \lambda_k + o(h) \; . \quad (16)$$

The probability for nuclide transmutation is:

$$P(i\rightarrow j) = h\cdot \lambda_l^{(i,j)} + o(h) \; . \quad (17)$$

The probability of formation of fission products is:

$$P(i\rightarrow j) = h\cdot \lambda_f^{(i)}\cdot p_{j,j} + o(h) \; . \quad (18)$$

The generating function of the process is:

$$f(x) = -\sum_k l_k^{(i)} \cdot x_i + \sum_{l=1}^{m-1} \sum_n l_n^{(i,l)} \cdot x_l + l_f^{(i)} \cdot (\sum_{l=m}^{L-1} p_{l,l+L} \cdot x_l \cdot x_{l+L} + \sum_{l=L+1}^{n} p_{l-L,l} \cdot x_l \cdot x_{l-L} + p_{L,L} \cdot (x_L)^2). \quad (19)$$

The generating function of the number of particles is:

$$F_i(t,x) = P\langle m(t) \,|\, m(0) = d \rangle \cdot x\,. \quad (20)$$

The differential equation for the generating functions is:

$$\frac{dF_i(t,x)}{dt} = f_i(F_1(t,x), F_2(t,x), \ldots)\,, \quad (21)$$

or

$$\frac{dF_i(t,x)}{dt} = \sum_k f_k(x) \cdot \frac{\P F_i(t,x)}{\P x_k}\,. \quad (22)$$

The formulae for mathematical expectations and central moments μ(t) are [1]

$$A_{ij} = \mathrm{M}\langle m_i(t) \,|\, m(0) = d_j \rangle\,, \quad (23)$$

$$B_{ij}^{(k)} = \mathrm{M}\langle m_i(t) \cdot m_j(t) \,|\, m(0) = d \rangle\,, \quad (24)$$

$$a_{ij} = \left.\frac{\P f_i(t,x)}{\P x_j}\right|_{x=1}, b_{ij}^{(k)} = \left.\frac{\P^2 f_i(t,x)}{\P x_j \cdot \P x_i}\right|_{x=1}, \quad (25)$$

$$A_{ij} = \left.\frac{\P F_i(t,x)}{\P x_j}\right|_{x=1}, \; B_{ij}^{(k)} = \left.\frac{\P^2 F_i(t,x)}{\P x_j \cdot \P x_i}\right|_{x=1}. \quad (26)$$

The result is equations whose form corresponds to the deterministic statement of the problem:

$$\frac{dA_{ij}}{dt} = \sum_{l=1}^{n} a_{il} \cdot A_{li}\,, \quad (27)$$

$$\frac{dB_{ij}^{(k)}}{dt} = \sum_{l=1}^{n} B_{ij}^{n}(t) \cdot a_{kl}(t) + \sum_{l_1,l_2=1}^{n} b_{lj}^{(k)} \cdot A_{l_1,i}(t) \cdot A_{l_2,j}(t)\,, \quad (28)$$

or

$$\frac{dA_{ij}}{dt} = \sum_{l=1}^{n} A_{il} \cdot a_{li} \,, \tag{29}$$

$$\frac{dB_{ij}^{(k)}}{dt} = \sum_{l=1}^{n} b_{ij}^{n}(t) \cdot A_{kl}(t) + \sum_{l_1,l_2=1}^{n} B_{lj}^{(k)} \cdot a_{l_1,i}(t) \cdot a_{l_2,j}(t) \,. \tag{30}$$

Then the mathematical expectation of the number of particles and the dispersion are determined as:

$$A_j(t) = \mathrm{M}\left\langle m_j(t) \middle| m(0) = (N_1,...) \right\rangle = \sum_{k=1}^{n} N_k \cdot A_{kj}(t) \,, \tag{31}$$

$$\frac{dA_j}{dt} = \sum_{l=1}^{n} A_l(t) \cdot a_{lj}(t) \,, \tag{32}$$

$$D_{ij}(t) = \sum_{l=1}^{n} N_l \cdot B_{ij}^{(l)}(t) \,. \tag{33}$$

$$\frac{dD_{ij}}{dt} = \sum_{l=1}^{n} \left[D_{lj} \cdot a_{li} + D_{il} \cdot a_{lj} \right] + \sum_{l=1}^{n} A_l \cdot b_{ij}^{(l)} \,. \tag{34}$$

The mathematical expectation for the number of particles may also be written as:

$$\mathrm{M}m_j = A_j \,. \tag{35}$$

The dispersion is given by:

$$\mathrm{D}m_{\mathrm{i}} = D_{ii} + A_i - \sum_{l=1}^{n} N_l \cdot A_{li}^2 \,. \tag{36}$$

The covariations matrix of the number of particles is given by:

$$\mathrm{cov}(m_i, m_j) = D_{ij} - \sum_{l=1}^{n} N_l \cdot A_{li} \cdot A_{il} \,. \tag{37}$$

The above formulae show that modelling using the small perturbations algorithm preserves the type of statistics up to second order central moments. This makes it possible to perform a linear error propagation in calculations using the Monte Carlo method.

The statistical uncertainty of the values to be calculated is given by a formula of the form:

$$s^2 = \frac{1}{N-1} \cdot \sum_{i=1}^{N} (x_i - \bar{x})^2 , \tag{38}$$

where N is the number of tests, x_i is an estimate of the value, and $\bar{x}$ is the mean value. The functionals employed as calculated rates of the processes are presented in the form of linear-fractional functionals:

$$f(m_1, m_2, m_3, \ldots, m_m) = \sum_{i=1}^{m} a_i \cdot m_i \Big/ \sum_{i=1}^{m} b_i \cdot m_i , \tag{39}$$

which corresponds to $s_{ef} = f(m_a, m_b) = m_a / m_b$ then the dispersion:

$$\mathbf{D}\, s_{ef} = \frac{m_a^2}{m_b^2} \cdot \left[\frac{\mathbf{D}\hat{m}_a}{m_a^2} + \frac{\mathbf{D}\hat{m}_b}{m_b^2} - \frac{2 \cdot \mathbf{M}(\hat{m}_a \cdot \hat{m}_b)}{m_a \cdot m_b} + 2 \right]. \tag{40}$$

For the linear chains considered earlier, we have:

$$r_l(t) = \sum_{ic} r_{ic}(t), \tag{41}$$

where l is the isotope index; ic is the number of the chain. Variations can be represented as:

$$\delta_\varepsilon \left(r_l(t) \right) = \sum_{ic} \delta_\varepsilon \left(r_{ic}(t) \right), \tag{42}$$

where $\delta_\varepsilon \left(r_n(t) \right)$ is the variation in the contribution of each chain from the parameter ε.

Then the probability of the sensitivity coefficient of the l-th nuclide in the ic-th chain for the m-th parameter can be written as:

$$h_m^{l,ic} = \frac{\partial r_l^{ic}}{\partial \varepsilon_m}, \tag{43}$$

where r_l^{ic} is the concentration of the l-th nuclide; ε_m is the m-th parameter; $h_m^{l,ic}$ is the sensitivity coefficient.

All the parameters in the Monte Carlo method are represented in the form

$$l_{ij} = \frac{\left\langle \vec{s}_l^{\,i} \vec{f} \right\rangle_m}{\left\langle \vec{f} \right\rangle_m}. \tag{44}$$

In the general case the solution is presented in operator form:

$$\vec{N}(T) = \hat{P}(T) \cdot \vec{N}(0), \tag{45}$$

where $\vec{N}(0)$ is the vector of the initial concentrations; $\vec{N}(T)$ is the concentration vector; $\hat{P}(T)$ is the linear operator of transmutation.

Then, over the time intervals:

$$\vec{N}^{\langle k \rangle} = \hat{P}^{\langle k-1 \rangle} \cdot \hat{P}^{\langle k-2 \rangle} \cdots \hat{P}^{\langle 0 \rangle} \cdot \vec{N}^{\langle 0 \rangle}. \tag{46}$$

Since the operators are piece-wise constant, we have for the relative variation with respect to the m-th parameter:

$$\frac{\partial \vec{N}^{\langle l \rangle}}{\partial \varepsilon_m} = \hat{P}^{\langle l-1 \rangle} \cdot \frac{\partial \vec{N}^{\langle l-1 \rangle}}{\partial \varepsilon_m} + \frac{\partial \hat{P}^{\langle l-1 \rangle}}{\partial \varepsilon_m} \cdot \vec{N}^{\langle l-1 \rangle}, \tag{47}$$

where $\frac{\partial \vec{N}^{\langle l \rangle}}{\partial \varepsilon_m}$ is the coefficient of sensitivity to the m-th parameter in the l-th interval; $\frac{\partial \hat{P}^{\langle i \rangle}}{\partial \varepsilon_m}$ is the functional derivative $\hat{P}^{\langle i \rangle}$.

The general solution is:

$$\begin{aligned} \frac{\partial N^{(k)}}{\partial \varepsilon_m} &= \frac{\partial \hat{P}^{(k)}}{\partial \varepsilon_m} \times P^{(k-2)} \cdots P^{(1)} \cdot N^{(0)} \\ &+ P^{(k)} \times \frac{\partial P^{(k-1)}}{\partial \varepsilon_m} \times P^{(k-2)} \cdots P^{(1)} \cdot N^{(0)} + P^{(k)} \times P^{(k-1)} \cdots P^{1} \cdot \frac{\partial N^{(0)}}{\partial \varepsilon_m}. \end{aligned} \tag{48}$$

The variation may be determined as

$$\delta_m(\vec{N}(t)) = \frac{\partial \vec{N}(t)}{\partial \varepsilon_m} \cdot \sigma_{\varepsilon_m}, \tag{49}$$

where σ_{ε_m} is the mean square deviation of the m-th parameter; $\frac{\partial \vec{N}(t)}{\partial \varepsilon_m}$ is the coefficient of sensitivity; $\delta_m(\vec{N}(t))$ is the absolute value of the mean square deviation.

The square of the deviation may be represented in the form

$$s_m^2(r_l(t)) = \frac{\delta_m(r_l(t))}{r_l(t)} \cdot \frac{\delta_m(r_l(t))}{r_l(t)} + \sum_k \operatorname{cov}(r_l(t), r_k(t)) \cdot \left| \frac{\delta_m(r_l(t))}{r_l(t)} \right| \cdot \left| \frac{\delta_m(r_k(t))}{r_k(t)} \right|. \tag{50}$$

Thus, the coefficients in the model of nuclide transmutations are calculated as integrals of the corresponding values obtained in the steady-state particle transport model. If we consider these coefficients as probability density functions of the corresponding transmutations and

describe the nuclide kinetics by a random branching process, distribution moments of the nuclide concentrations in reactor materials at different moments of time will go to form a series of computable quantities. However, the form of the equations does not change with transition from a deterministic description to a random process model, i.e. the algorithms and programs for calculating the nuclide kinetics in the approximation of the branching process are equally suitable for calculations of both deterministic and random systems. The method, based on the approximation of linear error propagation, assumes that the value of the statistical uncertainty of the result is small; deviations of the solution are small; corrections to the neutron flux and nuclide burnup rates are small; and each new recourse to programs modelling neutron transfer is statistically independent of the previous one.

SOME NUMERICAL RESULTS

A package of programs called PATRICK (Perturbed Analytical Treatment of the Reactor Inventory Modelling in the Condensed Parameters of Kinetics) has been developed. It is constructed on the basis of a mathematical model assuming conditional segregation of different physical processes. The calculation of an operating cycle of the nuclear system is performed by means of successive recalculation of the steady-state neutron and photon fields and the corresponding rates of nuclear processes. The proposed algorithms are applicable for the most general statement of the problem without substantial restrictions on the type of modelled nuclear system, except that the basic transmutations of nuclides are determined by neutron and photon nuclear reactions in the middle and low energy range (up to ~20 MeV). Despite the fact that the above processes in the nuclear system relate to the type of so-called neutron controlled processes, the problem can also be easily generalised to a consideration of other types of particles, provided that the sense of the spectral calculation and the algorithm for introducing the controlling parameters is changed. The changing of the reactor control algorithm and the spectral calculation does not change the form of the calculatory scheme and the formal construction of the kinetic model. The methods and algorithms of the program package provide a means of performing theoretical investigations associated with the modelling of the operating cycle of a nuclear system in real geometry with the aid of precision programs for calculating neutron and photon distributions.

The package of programs is intended for solving various problems associated with variations in the nuclide composition of materials in nuclear systems. In particular, it is possible to single out four principal tasks for which the proposed methods and programs may be employed.

- For precise calculation of the nuclide composition for a given regime of the nuclear system. For calculating the functionals of nuclide concentrations such as breeding capacity, activity and power density in irradiated materials, potential danger coefficients, etc. For calculating the nuclide composition with the aid of the Monte Carlo method taking the statistical error of the result into account.

- For analysing the errors in calculations of nuclide composition and its functionals associated with errors in the initial data and the calculation models by the small perturbation method. For solving inverse problems, i.e. questions of planning the supply of nuclear data.

- For solving optimisation problems in the design of special-purpose equipment intended for producing or eliminating specific nuclides, etc. This also includes problems of optimising the operating conditions of equipment with a view to reducing the toxicity of unloaded fuel or certain constructional elements.

- For analysing nuclear power fuel cycles, and modelling and optimising material flows in a power system.

With the aid of modules of the PATRICK package of programs one can use nuclide transmutation rates obtained in the calculation of steady-state neutron and photon fields for modelling changes in the composition of materials of the power plant. For generating libraries of nuclide transmutation chains, estimating the accuracy of calculation and preliminary selection of the spatial calculatory nodes and the time interval, one uses the perturbation theory. When using the Monte Carlo method, the package of programs and the methods developed enable one to estimate the statistical error of the calculation of the nuclide concentrations determined by the statistical errors in the modelling of the neutron and photon fluxes. Apart from analysis of the errors, the method of small perturbations is employed for calculating the effective neutron flux and modelling the cyclic chains of transmutation of nuclides under irradiation. The PATRICK programs may be used for analysing the stability of equilibrium points in investigations of nuclear power fuel cycles. The programs and methodology on which the PATRICK package is based have been developed with an eye to the further development of the soft and hardware for research in the field of nuclear engineering and particle transport theory.

Using the package of programs, it is possible to formulate certain requirements for the initial data, for example in research on transmutation concepts in accelerator-driven systems.

Here it should be remembered that the basis for formulating these requirements is the statement of the systems analysis problem. When considering the question of using an accelerator-controlled reactor-burner for nuclear waste, the following points need to be emphasised:

- the course of the investigations it is necessary to identify the contribution of neutrons from the evaporation-spallation reaction to the transmutation of nuclides;

- it is necessary to take into account the principal differences in the models of nuclear processes in the target of the accelerator and in the nuclear reactor;

- Due to the fact that in the accelerator target the nuclear processes are mainly described by the Monte Carlo method, it is necessary to model the statistical uncertainty in the computed nuclide concentrations.

Tables 1 and 2 show the changes in the nuclide vector in the model of an accelerator controlled system with thorium and minor actinides, while Tables 3 and 4 show the corresponding sensitivity coefficients.

Table 1 Results of calculating the nuclide concentrations in a thorium reactor with accelerator

	0 days	100 days	σ	Relative value
Th^{230}	$3{,}62\cdot10^{-8}$	$3{,}65\cdot10^{-8}$	$4{,}82\cdot10^{-11}$	0,13%
Th^{231}	0	$1{,}69\cdot10^{-9}$	$8{,}39\cdot10^{-11}$	4,98%
Th^{232}	$3{,}62\cdot10^{-3}$	$3{,}57\cdot10^{-3}$	$2{,}45\cdot10^{-6}$	0,07%
Pa^{231}	0	$1{,}01\cdot10^{-7}$	$5{,}05\cdot10^{-9}$	4,99%
U^{232}	0	$7{,}10\cdot10^{-9}$	$4{,}74\cdot10^{-10}$	6,68%
U^{233}	0	$2{,}97\cdot10^{-5}$	$1{,}48\cdot10^{-6}$	4,98%
U^{234}	0	$4{,}90\cdot10^{-7}$	$3{,}05\cdot10^{-8}$	6,22%
Energy	0	$2{,}82\cdot10^{-4}$	$1{,}94\cdot10^{-5}$	6,90%

Table 2 Results of calculating the nuclide concentrations in a reactor with accelerator loaded with minor actinides

	0 days	100 days	σ	Relative value
U^{234}	$1{,}34\cdot10^{-5}$	$1{,}32\cdot10^{-5}$	$1{,}58\cdot10^{-8}$	0,12%
U^{235}	$2{,}28\cdot10^{-6}$	$2{,}44\cdot10^{-6}$	$1{,}62\cdot10^{-8}$	0,66%
U^{236}	$2{,}93\cdot10^{-6}$	$2{,}93\cdot10^{-6}$	$3{,}85\cdot10^{-9}$	0,13%
Np^{237}	$1{,}51\cdot10^{-4}$	$1{,}38\cdot10^{-4}$	$3{,}97\cdot10^{-7}$	0,29%
Pu^{238}	$1{,}57\cdot10^{-4}$	$1{,}59\cdot10^{-4}$	$5{,}17\cdot10^{-7}$	0,32%
Pu^{239}	$8{,}10\cdot10^{-4}$	$7{,}34\cdot10^{-4}$	$2{,}15\cdot10^{-6}$	0,29%
Pu^{240}	$8{,}97\cdot10^{-4}$	$8{,}83\cdot10^{-4}$	$1{,}35\cdot10^{-6}$	0,15%
Pu^{241}	$3{,}26\cdot10^{-4}$	$3{,}08\cdot10^{-4}$	$1{,}54\cdot10^{-6}$	0,50%
Pu^{242}	$4{,}02\cdot10^{-4}$	$3{,}99\cdot10^{-4}$	$4{,}45\cdot10^{-7}$	0,11%
Am^{241}	$1{,}42\cdot10^{-4}$	$1{,}33\cdot10^{-4}$	$4{,}15\cdot10^{-7}$	0,31%
Am^{242m}	$6{,}85\cdot10^{-6}$	$7{,}71\cdot10^{-6}$	$8{,}94\cdot10^{-8}$	1,16%
Am^{243}	$2{,}05\cdot10^{-4}$	$2{,}01\cdot10^{-4}$	$5{,}34\cdot10^{-7}$	0,27%
Cm^{242}	$6{,}19\cdot10^{-6}$	$1{,}03\cdot10^{-5}$	$2{,}27\cdot10^{-7}$	2,19%
Cm^{243}	$2{,}93\cdot10^{-6}$	$2{,}71\cdot10^{-6}$	$1{,}41\cdot10^{-8}$	0,52%
Cm^{244}	$1{,}06\cdot10^{-4}$	$1{,}11\cdot10^{-4}$	$4{,}53\cdot10^{-7}$	0,41%
Cm^{245}	$1{,}63\cdot10^{-5}$	$1{,}87\cdot10^{-5}$	$1{,}72\cdot10^{-7}$	0,92%
Cm^{246}	$1{,}08\cdot10^{-5}$	$1{,}09\cdot10^{-5}$	$1{,}18\cdot10^{-8}$	0,11%
Cm^{247}	$1{,}30\cdot10^{-6}$	$1{,}32\cdot10^{-6}$	$5{,}68\cdot10^{-9}$	0,43%
Cm^{248}	$6{,}52\cdot10^{-7}$	$6{,}57\cdot10^{-7}$	$8{,}11\cdot10^{-10}$	0,12%
Energy		$2{,}32\cdot10^{-2}$	$5{,}28\cdot10^{-4}$	2,27%

Table 3 Sensitivity coefficients in the problem with thorium

Process	Capture	Fission	n,2n	n,3n
Th^{228}				
U^{234}	$-9{,}3\cdot10^{-21}$	$-2{,}4\cdot10^{-21}$	$2{,}26\cdot10^{-22}$	$1{,}13\cdot10^{-18}$
U^{236}	$7{,}63\cdot10^{-31}$	$-9{,}6\cdot10^{-34}$	$1{,}45\cdot10^{-32}$	$1{,}33\cdot10^{-30}$
Pu^{240}	0	0	0	$5{,}61\cdot10^{-45}$
Th^{229}				
U^{235}	$-6{,}7\cdot10^{-27}$	$-2\cdot10^{-26}$	$8{,}92\cdot10^{-27}$	$1{,}19\cdot10^{-24}$
Pu238	$-3{,}8\cdot10^{-34}$	$-4{,}1\cdot10^{-34}$	$6{,}22\cdot10^{-34}$	$1{,}41\cdot10^{-32}$
Pu^{239}	$-6{,}8\cdot10^{-42}$	$-1{,}7\cdot10^{-41}$	$1{,}95\cdot10^{-40}$	$2{,}25\cdot10^{-39}$
Pu^{240}	0	0	0	$1{,}4\cdot10^{-45}$
Th^{230}				
Th^{232}	$-5{,}3\cdot10^{-12}$	$-9\cdot10^{-14}$	$-1{,}2\cdot10^{-14}$	$8{,}13\cdot10^{-10}$
U^{236}	$3{,}94\cdot10^{-26}$	$-7{,}8\cdot10^{-29}$	$3{,}55\cdot10^{-29}$	$1{,}77\cdot10^{-25}$
Pu^{240}	$1{,}28\cdot10^{-40}$	$-8{,}9\cdot10^{-43}$	$4{,}2\cdot10^{-44}$	$9{,}11\cdot10^{-40}$
Pa^{231}				
Pa^{233}	$-1{,}2\cdot10^{-14}$	$-3{,}1\cdot10^{-16}$	$-1{,}9\cdot10^{-18}$	$9{,}83\cdot10^{-13}$
Pu^{240}	$-3{,}4\cdot10^{-43}$	$-1{,}3\cdot10^{-43}$	0	$7{,}99\cdot10^{-43}$
U^{232}				
U^{234}	$-5\cdot10^{-17}$	$-1{,}3\cdot10^{-17}$	$1{,}25\cdot10^{-18}$	$5{,}83\cdot10^{-15}$
U^{236}	$4{,}88\cdot10^{-27}$	$-6{,}1\cdot10^{-30}$	$9{,}06\cdot10^{-29}$	$7{,}8\cdot10^{-27}$
Pu^{240}	$5{,}7\cdot10^{-42}$	$-4{,}1\cdot10^{-44}$	$1{,}4\cdot10^{-45}$	$4{,}04\cdot10^{-41}$

Table 4 Sensitivity coefficients in the problem with minor actinides

	Capture	Fission	n,2n	n,3n
Am^{239}				
Am^{241}	$-1{,}84\cdot10^{-15}$	$-1{,}48\cdot10^{-16}$	$-4{,}92\cdot10^{-20}$	$2{,}13\cdot10^{-14}$
Cm^{243}	$1{,}06\cdot10^{-24}$	$-2{,}77\cdot10^{-25}$	$6{,}16\cdot10^{-28}$	$4{,}80\cdot10^{-24}$
Am^{240}				
Am^{242m}	$-4{,}15\cdot10^{-16}$	$-3{,}54\cdot10^{-15}$	$1{,}11\cdot10^{-17}$	$2{,}24\cdot10^{-14}$
Am^{242}	$-6{,}95\cdot10^{-20}$	$-4{,}61\cdot10^{-19}$	$6{,}58\cdot10^{-20}$	$1{,}37\cdot10^{-15}$
Cm^{243}	$4{,}38\cdot10^{-22}$	$-1{,}17\cdot10^{-22}$	$2{,}63\cdot10^{-25}$	$2{,}09\cdot10^{-21}$
Am^{241}				
Cm^{243}	$6{,}82\cdot10^{-15}$	$-1{,}77\cdot10^{-15}$	$3{,}92\cdot10^{-18}$	$3{,}03\cdot10^{-14}$
Am^{242m}				
Cm^{243}	$2{,}34\cdot10^{-17}$	$-7{,}51\cdot10^{-18}$	$1{,}86\cdot10^{-20}$	$1{,}95\cdot10^{-16}$
Cm^{241}				
Cm^{243}	$-2{,}15\cdot10^{-16}$	$-1{,}89\cdot10^{-15}$	$5{,}35\cdot10^{-18}$	$2{,}48\cdot10^{-14}$

It is clear that the increase in the statistical uncertainty (the calculation was performed by the Monte Carlo method) is limited.

It is clear that the influence of inelastic processes involving fast neutrons in accelerator-controlled systems is greater, but the sensitivity coefficients obtained show that the main contribution is made by the same neutron reactions as in conventional fast reactors.

Next example of applications of sensitivity analysis is estimation of requirements to accuracy of decay parameters data of construction material of nuclear systems. It can be useful in systematic approach of nuclear industry strategies analysis. Thus it was considered radiation characteristics of irradiated in very intensive neutron flux stainless steel. Value of neutron flux is $1.2 \cdot 10^{16} \frac{neutr}{cm^2 \cdot \sec}$. Spectrum of neutrons corresponds to one variant of sodium cooled reactor spectrum [3]. Material in the model irradiated for three years and cooled for next ten years. An error in each of probability of decay density for any nuclide can results an error in complete activity of material directly (by variation of chosen nuclide concentration and its contribution in complete activity) and indirectly (by variation of its daughter nuclides concentrations). Thus in table 5 two part of contributions in complete activity of irradiated steel are shown. First part is the complete contribution and second part is the indirect contribution.

Table 5 Sensitivity coefficients of activity in the problem with steel irradiation in very intensive neutron flux

	After irradiation		After cooling	
specific activity,	$1{,}83 \cdot 10^{12}$ Bk/cm^3		$1{,}64 \cdot 10^{9}$ Bk/cm^3	
	complete contribution	indirect contribution	complete contribution	indirect contribution
V^{49}	$-2{,}36 \cdot 10^{-10}$	0	$-4{,}71 \cdot 10^{-9}$	0
Cr^{51}	$-5{,}04 \cdot 10^{-2}$	$-9{,}16 \cdot 10^{-10}$	$-4{,}80 \cdot 10^{-10}$	$-4{,}80 \cdot 10^{-10}$
Mn^{54}	$-8{,}86 \cdot 10^{-6}$	$-1{,}21 \cdot 10^{-9}$	$-7{,}21 \cdot 10^{-5}$	$-1{,}87 \cdot 10^{-15}$
Mn^{56}	-0,7495	$-1{,}39 \cdot 10^{-7}$	$-1{,}08 \cdot 10^{-5}$	$-1{,}08 \cdot 10^{-5}$
Fe^{55}	$-1{,}34 \cdot 10^{-3}$	$-2{,}97 \cdot 10^{-5}$	-2,24139	$-1{,}06 \cdot 10^{-10}$
Fe^{59}	$-2{,}17 \cdot 10^{-3}$	$-6{,}18 \cdot 10^{-5}$	$-2{,}47 \cdot 10^{-3}$	$-2{,}47 \cdot 10^{-3}$
Co^{58}	$-5{,}63 \cdot 10^{-10}$	$-1{,}59 \cdot 10^{-11}$	$-4{,}45 \cdot 10^{-10}$	$-4{,}45 \cdot 10^{-10}$
Co^{60}	$-4{,}61 \cdot 10^{-7}$	$-5{,}84 \cdot 10^{-20}$	$-4{,}93 \cdot 10^{-3}$	$-6{,}14 \cdot 10^{-17}$
Co^{60m}	$-7{,}12 \cdot 10^{-5}$	$-3{,}72 \cdot 10^{-6}$	$-1{,}12 \cdot 10^{-3}$	$-1{,}12 \cdot 10^{-3}$
Ni^{59}	$-2{,}27 \cdot 10^{-11}$	$-3{,}28 \cdot 10^{-13}$	$-5{,}36 \cdot 10^{-7}$	$-9{,}47 \cdot 10^{-12}$
Ni^{63}	$-6{,}78 \cdot 10^{-7}$	$-1{,}08 \cdot 10^{-9}$	$-1{,}48 \cdot 10^{-2}$	0
Cu^{64}	$-4{,}32 \cdot 10^{-7}$	0		
Mo^{93}	$-1{,}81 \cdot 10^{-11}$	0	$-4{,}23 \cdot 10^{-7}$	0
Mo^{99}	-0,18686	$-6{,}42 \cdot 10^{-8}$	$-7{,}38 \cdot 10^{-5}$	$-7{,}38 \cdot 10^{-5}$
Tc^{98}	$-2{,}62 \cdot 10^{-21}$	0	$-8{,}98 \cdot 10^{-17}$	0
Tc^{99}	$-9{,}95 \cdot 10^{-14}$	$-4{,}80 \cdot 10^{-20}$	$-2{,}51 \cdot 10^{-9}$	$-5{,}37 \cdot 10^{-17}$

CONCLUSION

1. A method and algorithm are developed for computing the sensitivity coefficients and calculating the effect of small perturbations in the context of analytical solution of nuclide kinetics equations.

2. An algorithm and methodology are proposed for extending the method of analytical solution of nuclide kinetics equations (in the form of Bateman equations) to problems with weak non-linearity and the presence of neutron and photon radiation. This also includes problems of modelling variations in the composition of materials of a nuclear system, where in the course of irradiation a certain given functional is preserved, for example, the power of the whole system. Sensitivity coefficients are employed in this algorithm for correcting the solution in the event of variations in the neutron flux which, in their turn, are determined by the maintenance of the concentration of a conditionally specified pseudo-nuclide corresponding to the integral from the given functional. It should be noted that both solutions without corrections and also the corrections (and sensitivity coefficients) are calculated from analytical dependencies which rules out the accumulation of a computational error.

3. A method is developed for estimating the statistical uncertainty of nuclide concentrations in the case of statistically distributed kinetics parameters. The statistical error arises due to the need to carry out calculations of the operating cycle of nuclear systems with the aid of the Monte Carlo method. For estimating the statistical uncertainty, we use the method of linear error propagation and the algorithms for computing the coefficients of sensitivity of the result to changes in the nuclide kinetics parameters. It is shown that algorithms, developed for deterministic description of the nuclide transmutation process, can be used for calculating the distribution moments of nuclide concentrations. For calculating the influence of small statistical deviations of the kinetics parameters (rates of processes), an analysis of the correlations of deviations is included in the algorithm.

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