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Research Article

The effect of errors in the neutron flux density on the uncertainties of nuclear concentrations of nuclides arising during the calculation of fuel burnup in cells with different neutron spectra*

Aleksandr N. Pisarev[1], Valery V. Kolesov[1], Dmitry V. Kolesov[2]

1 *National Research Center "Kurchatov Institute", 1 Akademika Kurchatova Sq., 123182, Moscow, Russia*

2 *FSBSI "Research Institute of General Pathology and Pathophysiology", 8 Baltiyskaya St., 125315, Moscow, Russia*

Corresponding author: Aleksandr N. Pisarev (a.n.pisarev93@gmail.com)

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Abstract

Computational studies have been carried out showing the complex time dependence of uncertainties in nuclear concentrations of various nuclides arising from the propagation of the neutron flux density errors in the burnup calculation process in cells with different neutron spectra on the above errors.

It is found that these uncertainties not only depend on the burnup time in a complex way, but also depend on the spectrum of the cell. The variants of the cell with thermal and fast neutron spectra were considered.

The calculations were performed using the VisualBurnOut program (Kolesov et al. 2009), which makes it possible to estimate these uncertainties arising due to errors in the input parameters of the burnup problem (reaction rates, neutron flux density, etc.).

The influence of the number of calculated burnup points on the results of burnup calculations by the Monte Carlo method was investigated. Uncertainties arising in nuclear concentrations at intermediate calculation steps due to errors in nuclear concentrations appearing at the previous step were taken into account in the calculations.

Keywords

Reactor plant, burnup calculations, uncertainties in nuclear data, uncertainties in nuclide nuclear concentrations, Monte Carlo method, neutron spectrum

Introduction

Estimation of errors for different physical quantities obtained as the result of calculations due to errors (errors will universally hereafter mean to understand root-mean-square deviations) in initial data, e.g., nuclear physical constants, is one of the most important problems in neutronic calculation.

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In Monte Carlo burnup calculations, the burnup period is divided by a finite number of disjoint time steps. At the beginning of each burnup time step, the Monte Carlo method is used to calculate microscopic reaction rates. The calculated microscopic reaction rates are introduced and used for solving isotopic kinetics equations to determine the nuclear concentrations of all nuclides at the end of the burnup time step.

The reaction rates estimated by the Monte Carlo method at the beginning of each burnup time step require to contain errors arising due to errors in microscopic cross-sections and initial nuclear concentrations of nuclides, as well as in the static error of the Monte Carlo calculations. These lead to errors in the nuclear concentrations obtained in solving burnup equations at the end of the burnup time step. Therefore, the errors in nuclear concentrations of nuclides and estimated reaction rates propagate to other burnup time steps. To estimate the propagation of errors during the burnup period, it is required to use many time steps and undertake multiple Monte Carlo calculations.

A great number of studies were undertaken for burnup calculations using Monte Carlo codes, such as MONTEBURNS (Trellue 2006), MVP-BURN (Okumura et al. 2000), MCNPX0CINDER90 (Fensin et al. 2006), McCARD (Shim and Kim 2002), and others. However, there are not so many studies (Takeda et al. 1999, Tohjoh et al. 2006, Garcia-Herranz et al. 2008, Park et al. 2011, Rochman et al. 2012, Quentin Newella and Charlotta Sanders 2015, Minamigawa et al. 2019) dealing with quantitative estimations of nuclear concentration errors in isotopic kinetics calculations and their propagation in the fuel burnup process.

In (Pisarev and Kolesov 2020), a complex time dependence is shown for nuclear concentration errors for different nuclides arising in the propagation of single-group constant or neutron flux density errors in the process of calculating burnup in a thermal spectrum. This study aims to estimate the influence of errors in defining the neutron flux density in fast and thermal neutron spectra on the nuclear concentration errors in the burnup process.

The proposed methodology for estimating the effect of errors in the burnup problem input parameters on the errors in nuclear concentrations obtained in the burnup process has been justified by the results obtained in (Kolesov et al. 2017). That study estimated the effect of errors in the burnup problem input parameters on the nuclear concentration errors obtained due to this in the burnup process using a statistical approach. For an input parameter, the error (root-mean-square deviation) for which was assumed to be distributed in a logarithmically normal way, its specific value was drawn repeatedly and the burnup problem was solved. As the result of the burnup problem solution, a distribution of the nuclear concentrations of nuclides was obtained and the respective error (root-mean-square deviation) was determined. The results of the studies have shown that the root-mean-square deviations of nuclear concentrations obtained statistically coincide with the nuclei concentration errors obtained in a variation method in which only two calculations were enough: with the input parameter minus the root-mean-square deviation, and with the input parameter plus the root-mean-square deviation. The difference between these two values of nuclear concentrations coincides for the most part with the root-mean-square deviation obtained in the statistical approach.

Calculation results

To investigate the effect of errors in defining the neutron flux density on the nuclear concentrations of nuclides, a PWR reactor cell model was studied representing a three-zone square cell (mesh spacing of 1.3127 cm) with MOX fuel (Stepanek and Vontobel 1987). The fresh fuel, cladding and moderator compositions are given in Table 1.

Table 1. PWR cell structure

N×10^{24} nuclei/cm^3	**Fuel (PuO_2+UO_2), T=900K**	**Cladding (zircaloy), T=620K, external diameter 0.475 cm, thickness 0.065 cm**	**Moderator (H_2O), T=575K**
^{234}U	2.7043E-7		
^{235}U	5.6570E-5		
^{238}U	2.2286E-2		
^{238}Pu	4.5941E-7		
^{239}Pu	8.5640E-4		
^{240}Pu	5.4669E-5		
^{241}Pu	2.7221E-6		
^{16}O	4.5180E-7		
Zr (natural)		3.8657E-2	
Fe (natural)		1.3345E-4	
Cr (natural)		6.8254E-5	
H			4.8414E-2
O			2.4213E-2
^{10}B			4.7896E-6
^{11}B			1.9424E-5

A fixed flux density error of 10% was used for the calculations. All of the results discussed below were obtained for the given flux density error. In reality, this error is much smaller and varies as a function of burnup. Therefore, this error can be assumed to be a certain model error. The actual (experimental) error can be determined, e.g., as the result of experiments to determine the neutron flux density in actual benchmarks.

The calculations were performed based on the VisualBurnOut code (Kolesov et al. 2009) using Monte Carlo calculated single-group reaction rates and fluxes.

To avoid the effects of the initial fuel composition, the same PWR reactor cell was selected for investigating the fast spectrum effect but only with a hard spectrum. For a harder spectrum, the geometry and the concentration of hydrogen in the moderator were changed.

Fig. 1 presents a distribution of the neutron spectrum portions for the initial thermal cell and for a fast cell for three energy intervals showing that the spectrum is thermal in the former case and is fast in the latter case.

The results obtained for the root-mean-square deviations in the nuclear concentrations of nuclides for the fast spectrum were compared with the results obtained in (Pisarev and Kolesov 2020).

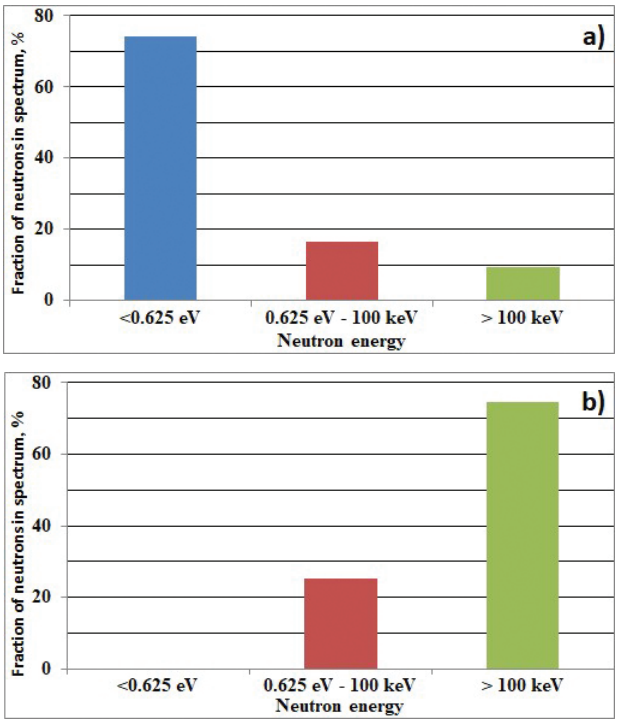

Figure 1. Thermal neutron spectrum (**a**) and fast neutron spectrum (**b**).

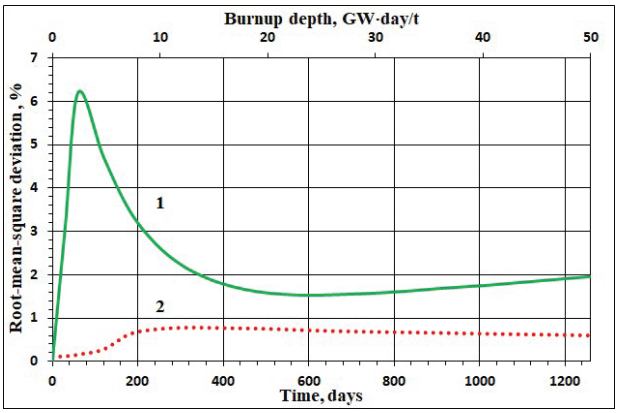

Figure 2. Root-mean-square deviation (errors) in the nuclear concentration of ^{241}Am: 1 – thermal spectrum; 2 – fast spectrum.

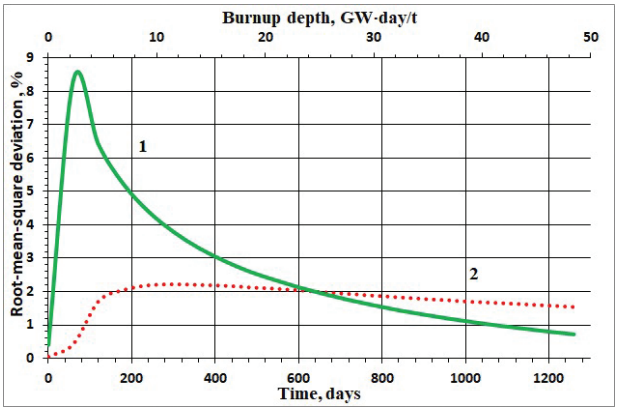

Figure 3. Root-mean-square deviation (errors) in the nuclear concentration of ^{241}Pu: 1 – thermal spectrum; 2 – fast spectrum.

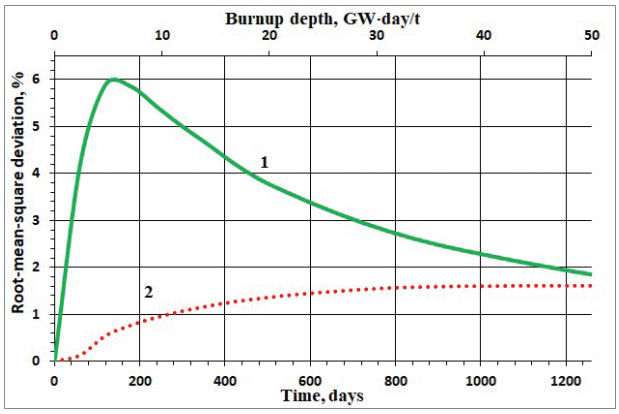

Figure 4. Root-mean-square deviation (errors) in the nuclear concentration of ^{242}Pu: 1 – thermal spectrum; 2 – fast spectrum.

Table 2. Nuclear concentrations of nuclides and their errors as of the reactor life end with a 10% flux density error

Nuclide	Thermal spectrum		Fast spectrum	
	Error, %	N×10^{24} nuclei/cm^3	Error, %	N×10^{24} nuclei/cm^3
^{137}Cs	0.51	6.5526E-5	0.51	6.7441E-5
^{155}Eu	0.74	6.2419E-7	0.68	1.6952E-6
^{155}Gd	5.71	1.2394E-8	0.18	3.4383E-7
^{157}Gd	1.92	2.3097E-8	0.51	7.0382E-7
^{158}Gd	0.85	2.0824E-6	0.58	4.5752E-7
^{234}U	1.36	1.7528E-7	0.38	2.4967E-7
^{235}U	2.18	2.0311E-5	1.71	2.6407E-5
^{236}U	1.76	6.6135E-6	2.11	6.0805E-6
^{238}U	0.05	2.1544E-2	0.20	2.0185E-2
^{237}Np	1.05	3.1880E-6	1.59	7.0853E-6
^{238}Pu	0.93	3.8438E-6	1.48	1.9074E-6
^{239}Pu	0.94	2.7440E-4	0.68	1.7051E-3
^{240}Pu	0.43	1.8115E-4	1.49	2.0610E-4
^{241}Pu	0.72	1.0621E-4	1.54	1.5168E-5
^{242}Pu	1.85	3.6946E-5	1.61	1.4526E-6
^{241}Am	1.96	5.3795E-6	0.60	1.1407E-6
^{242m}Am	0.97	1.1430E-7	2.06	1.5666E-8
^{243}Am	2.12	8.7295E-6	1.95	9.6828E-8
^{242}Cm	3.80	1.5823E-6	3.90	4.9779E-8
^{243}Cm	2.77	1.4596E-8	2.88	1.9457E-9
^{244}Cm	3.03	3.7437E-6	2.48	1.6731E-8
^{245}Cm	3.18	3.5184E-7	2.65	8.7577E-10

Figs 2 through 4 show the nature of the change in the nuclear concentration errors for ^{241}Am, ^{241}Pu and ^{242}Pu in the course of the reactor life for a thermal spectrum and a fast spectrum. These nuclides are some of few the error propagation nature for which depends on the neutron spectrum. Most nuclides behave in a similar way in the course of time. The difference consists only in the numerical value of the error as of the life end as shown in Table 2.

A trend is observed for most nuclides towards smaller errors in the transition between the thermal neutron spectrum to the fast neutron spectrum. There are however nuclides for which an opposite trend is observed (^{236,238}U, ^{237}Np, ^{240,241}Pu,^{242m}Am,^{242,243}Cm). This will be investigated further.

The error becomes larger for isotopes with relatively small nuclear concentrations ($^{242–245}$Cm, ^{241}Am, ^{243}Am). The nuclear concentration error for ^{238}U is very small due to a large nuclear concentration of this isotope. Errors for

fission products are largely below 1%. An exclusion is gadolinium isotopes which have a large cross-section in the thermal spectrum.

Influence of the number of calculated burnup points on errors in the nuclear concentrations of nuclides

In Monte Carlo burnup calculations, the errors in the model's input parameters propagate to the nuclear concentrations of nuclides through an exponential function. In these conditions, there is a probability that the errors in the nuclear concentrations of nuclides depend on the number of the calculated burnup points.

Table 3. Errors in nuclear concentrations of nuclides depending on the number of calculated burnup points with a 10% flux density error

Burnup depth, GW·day/t	Number of calculated burnup points								
	44			22			11		
	Errors in nuclear concentrations of nuclides, %								
	^{235}U	^{239}Pu	^{241}Am	^{235}U	^{239}Pu	^{241}Am	^{235}U	^{239}Pu	^{241}Am
16	0.85	0.84	0.94	1.21	1.18	1.34	1.69	1.66	1.78
32	1.18	0.89	1.16	1.69	1.26	1.63	2.36	1.74	2.32
48	1.49	0.79	1.37	2.11	1.08	1.96	2.97	1.49	2.66

The errors in nuclear concentrations were estimated depending on the number of burnup steps. The root-mean-square deviations in the nuclear concentrations of ^{235}U, ^{239}Pu and ^{241}Am obtained for different numbers of burnup steps (11, 22 and 44) are presented in Table 3. It can be seen from the table that the errors of nuclear concentrations in the considered investigation range for the influence of the number of steps diminish in $2^{1/2}$ increments. Most likely, this is valid for a relatively small number of steps. No asymptotic dependence of errors (when the number of steps grows) has been studied. This will be done later.

The cost of calculations in actual Monte Carlo calculations depends greatly on the costs concerned with the total number of neutron histories by the Monte Carlo method when preparing single-group cross-sections at each burnup step. One cannot therefore increase infinitely the number of calculated burnup points but shall reasonably limit the calculation time. The obtained results of the error estimations depending on the number of steps make it possible to state that it is preferable to have a smaller number of calculated burnup points when it is not required to obtain high-accuracy results in estimation of errors and a larger number of calculated burnup points for cases, e.g., PIE (Post-irradiation Experiments), which require high-accuracy results in nuclear concentrations of nuclides. In both cases, we obtain an upper-bound estimate of the error.

Conclusions

Errors (root-mean-square deviations) in nuclear concentrations of nuclides caused by the error in defining the neutron flux density have been estimated for the thermal and fast neutron spectra. Errors in the nuclear concentrations of various nuclides obtained based on the thermal and fast spectra have been compared.

These comparisons have shown that the effects of the input data error propagation (for the neutron flux density in the given case) in Monte Carlo burnup calculations for a PWR thermal cell depend in a complex way on the neutron spectrum. Issues have been identified which require an additional investigation. It will be reasonable to analyze further the effect of errors in reaction rates for the thermal and fast spectra and find out which reactions have the greatest effect on the errors in concentrations of particular nuclides.

We have also checked the effect of the number of calculated burnup points on errors in the nuclear concentrations of nuclides. The root-mean-square deviation in the nuclear concentrations of nuclides in the considered investigation range for the effect of the number of steps has been found to diminish in $2^{1/2}$ increments. It therefore appears reasonable to undertake more studies to investigate the behavior of errors for a much larger number of steps.

It is planned to calculate the coefficients of sensitivity of nuclear concentrations to different nuclear data. This will make it possible to look into the issue of the behavior of nuclear concentration errors with different values of the input data errors.

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