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Research Article

A computer code for optimizing the neutronics model parameters based on results of reactor physics experiments*

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Abstract

The paper describes in brief the functional capabilities of a computer code for optimizing the neutronics model parameters (neutron data, technological parameters, and their covariance matrices) based on results of reactor physics experiments using conditional nonlinear multi-parameter optimization algorithms. The code's application scope includes adjustment of neutron constants, technological parameters and their covariance matrices based on integral measurement results, formulation of requiremen117198ts with respect to the neutron data uncertainties for achieving the target accuracies in calculation of the reactor functionals, and estimation of the reactor performance prediction accuracy, as well as the informativity and similarity metrics of reactor physics experiments with respect to each other and in relation to the target reactor system. The paper also considers some examples of using the code to refine the neutronics models of nuclear reactor and fuel cycle systems based on results of reactor physics experiments.

Keywords

reactor functionals, benchmark models, reactor physics experiments, neutron data, technological parameters, uncertainties, data assimilation

Introduction

Designs of innovative nuclear reactor and related fuel cycle components are optimized primarily for the purpose of improving the economic performance of systems and their competitive edge with regard for nuclear and radiation safety requirements. A realistic way to reduce the design tolerances and margins that define in the long run the economic efficiency and competitiveness of plants while ensuring, with no constraints, nuclear and radiation safety requirements is to minimize the variety of uncertainties in reactor characteristics associated with nuclear data and technological parameters which are mandatorily estimated in project design. The only way to reduce the uncertainties in prediction of the reactor physics performance is to take into account experimental data via using dedicated algorithms for transfer of these data into calculations known as *data assimilation*.

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However, as a rule, there is a problem of insufficient experimental data from measurements of neutronics performance for systems structurally similar to target designs (due to high cost of respective reactor physics experiments), this affecting the limitation of capabilities for justifying, in a comprehensive manner, the efficiency and safety of facilities under design. It will be timely in this connection to consider and transfer all currently available experimental information, obtained as part of alternative experimental programs, to the target facility which makes it possible to improve the accuracy of predicting the performance of innovative nuclear reactors and related fuel cycle systems while eliminating the need for additional expensive experiments. Improving the procedural and instrumental framework used to assimilate reactor physics experimental data for increasing the accuracy of predicting the reactor performance in conditions of insufficient experimental data is a timely scientific and practical task solving which allows reducing the design tolerances and margins and improving so the economic efficiency and competitive edge of plants under design.

The practically important example described above does not limit the application scope for the procedure to assimilate reactor physics experimental data in nuclear engineering: the procedure is also used to develop benchmark models for reactor physics experiments (a benchmark experiment is an experiment of a reference class with the minimal estimated uncertainties), plan new informative measurements, adjust neutron constants based on integral measurement results, update stationary and time-dependent neutronics models, estimate the uncertainties in reactor characteristics due to neutron data and technological parameters uncertainties, and determine the target accuracies of neutron data and the prediction accuracies for the neutronics performance of nuclear reactor and fuel cycle facilities.

There are multiple possible ways to implement the procedures for assimilating reactor physics experimental data, each with advantages and drawbacks of its own, which can be divided into two groups (see Table 1):

1) classical approaches dating back to the 1970s – unconstrained optimization (problem solving is reduced to a system of linear algebraic equations);
2) modern approaches – transition from unconstrained to constrained optimization problem statement (consideration of physical constraints and contradictory experimental data, possibility for implementing alternative adjustment strategies, availability of built-in mechanisms for checking the quality and how 'physical' are the solutions, etc.).

Despite the diversity of approaches and software tools for assimilation of reactor physics experimental data, work has been continuously under way to develop and improve these further for the purpose of providing, on their basis, the possibility for reducing uncertainties in the design performance of innovative reactor plants, improve the accuracies of predicting the nuclear safety parameters, identify the most required areas for the neutron data updating, etc.

One of such developed tools is a computer code for optimizing the parameters of neutronics models with regard for reactor physics experiment results – ONIX (Andrianov et al. 2022), the functional capabilities of which (including the key approximations, implemented algorithms, application scopes) are described below. It should be noted that the au-

Table 1. Approaches to neutronics data assimilation

Methods		
Classical approaches (*)	**Modern approaches (**)**	
Unconstrained optimization (ANL, CEA, JAEA, JSI, ORNL, IPPE, NIKIET) (***)	Stochastic methods (NRG) (****)	Constrained nonlinear multi-parameter optimization (SG46, LANL, INL, IATE MEPhI) (*****)
Implementation peculiarities, key assumptions		
Ease of implementation (reduction to solution of a system of linear algebraic equations)	No need for linearizing the neutronics model	Possibility for taking directly into account the requirements to updated data
Assumption of normally distributed initial parameters	Applicability for any types of initial parameters distributions	Possibility for 'contradictory' experiments to be used in the analysis
Linearization of the neutronics model via calculation of sensitivity coefficients	Possibility for contradictory experiments to be used in the analysis	Possibility for taking into account nonlinear effects Possibility for solving an 'inverse problem' to determine required accuracies of initial data
Limitations of the approach, requirements for computational algorithms		
No possibility for taking into account requirements to data to be adjusted	Higher requirements to the quality of initial covariance matrices	Higher requirements to the quality of initial covariance matrices
Requirement for excluding 'contradictory' experiments from the analysis	Requirement for using time-consuming algorithms for stochastic optimization and dispersion reduction methods	Requirement for using current algorithms for constrained nonlinear multi-parameter optimization
No built-in mechanisms for diagnosis of nonphysical solutions		
Requirement for undertaking an additional statistical analysis of initial and adjusted data		

(*) Conn et al. 2000, Usachev and Bobkov 1980, Nikolaev and Ryazanov 1974, Vankov and Voropaev 1974, Manturov 2017, Assessment of Existing Nuclear Data Adjustment Methodologies 2011, Palmiotti et al. 2015, Klimov 2015, Hoefer and Buss 2021, Rochman et al. 2016.
(**) Andrianov et al. 2022, Siefman et al. 2018, 2020, Castelluccio et al. 2021, Cabellos O 2021.
(***) Manturov 2017, Assessment of Existing Nuclear Data Adjustment Methodologies 2011, Palmiotti et al. 2015, Klimov 2015.
(****) Hoefer and Buss 2021, Rochman et al. 2016.
(*****) Andrianov et al. 2022, Siefman et al. 2018, Cabellos 2021.

thors do not provide in this paper a description of other software tools or an analysis of their respective advantages and drawbacks since this is beyond the scope of the current study.

Brief description of the ONIX code

Functionally, the ONIX code allows calculating optimal corrections for the initial neutronics model parameters (neutron data, technological parameters, and their covariance matrices), which minimize the calculation and experimental discrepancies (the objective function – a chi square – is discussed below), with regard for the user-defined requirements to data (e.g., bounds of model parameters adjustments) and the calculation accuracies of the reactor functionals (a set of constraints), determining the required data uncertainties for ensuring the target accuracy of the reactor functional calculation, estimating the bias in the calculated performance of target reactor system and their respective uncertainties when using adjusted initial data, calculating the set of informativeness indicators and similarity of reactor physics experiments to each other and with respect to the target system, and estimating the neutron data and technological uncertainty in the reactor performance.

Specific features of the ONIX code: direct implementation of algorithms for constrained nonlinear multi-parameter optimization (trust-region (TRM) family algorithms (Conn et al. 2000) are used, which are reliable and stable, have good convergence properties, and can be applied to ill-posed problems), this making it possible to implement different strategies for adjustment of initial data and their covariances based on integral measurement results with regard for the set of user requirements to the final set of neutron data and technological parameters, estimate the effects of the adjustments made on the reactor performance predictions, absence of limits for the number of the neutron data representation energy groups, and integration with modern data processing and visualization tools.

The optimization problem for reactor physics experimental data assimilation solved using the ONIX code can be formulated in general as follows. Let **E** be the vector of the values measured in the experiments, and **x** the vector of the parameters (neutron constants and/or technological parameters) that define the neutronics model used to calculate the quantities measured (**C**(**x**) is the vector of respective calculated values). Mathematically, the problem is reduced to finding the minimum of the objective function (chi square) with regard for the bounds imposed on the varying ranges of the model parameters and additional constraints that articulate the requirements to the quality of the model parameters:

$$\begin{cases} (\mathbf{x}-\mathbf{x}_0)^{\mathrm{T}}\mathbf{M}_x^{-1}(\mathbf{x}-\mathbf{x}_0)+(\mathbf{E}-\mathbf{C}(\mathbf{x}))^{\mathrm{T}}\left(\mathbf{W}^{\mathrm{T}}\mathbf{M}_E\mathbf{W}\right)^{-1}(\mathbf{E}-\mathbf{C}(\mathbf{x}))\to\min \\ h_i^{\min}\le x_i-x_{i0}\le h_i^{\max}\ (i=1,\ ...,\ N_x) \\ f_k^{\min}\le F_k(\mathbf{x},\mathbf{x}_0,\mathbf{E},\mathbf{C}(\mathbf{x}))\le f_k^{\max}\ (k=1,\ ...,\ K) \end{cases} \quad (1)$$

where $\mathbf{x_0}$ is the vector of the initial parameter values (neutron constants and/or technological parameters); h_i are the limits for the bias in parameters, x_i; F_k is the metric of calculation and experimental discrepancies for one or several measurements; f_k are the limits for F_k (*min* and *max* are the lower and the upper boundary respectively); **W** is the diagonal matrix of the experiment weights; and $\mathbf{M}_x$ and $\mathbf{M}_E$ are the covariance matrices of parameters and measurements respectively ($\mathbf{M}_{ii} = d_i$ (variance) for $i = j$; $\mathbf{M}_{ij} = \mathrm{cov}(x_i, x_j)$ for $i \neq j$).

One of the major difficulties encountered in the practical application of the procedure to assimilate reactor physics experimental data consists in the need for analyzing diversified measurements which are often found to be mutually contradictory. Considering such experimental data individually leads to opposite trends in the biases of **C**(**x**) and parameters of **x**. Procedures are built in the ONIX code for identifying contradictory experiments based on different statistical data (a total chi square and individual chi squares both with and without taking into account correlations, coefficients of correlations for different experiments, Ishikawa factor, etc.) NEA/NSC/R(2016)6 2017), as well as the possibility for regulating the contribution of each experiment to the objective function using a matrix of experiment weights, **W**.

The ONIX code implements as well traditional approaches to the neutron constants adjustment with regard for integral experiment results based on unconstrained optimization using the maximum likelihood and the generalized least square methods (Nikolaev and Ryazanov 1974; Vankov and Voropaev 1974; Usachev and Bobkov 1980; Manturov 2017). Additionally, the authors modification of such approaches was implemented based on the Lagrange multiplier method which makes it possible to ensure in the process of adjustment that the equality of calculation and experimental values is satisfied exactly (it makes sense to use this modification when adjusting jointly neutron constants and technological parameters, e.g., when developing benchmark models for reactor physics experiments).

The ONIX code allows estimating different metrics of the informativeness indicators and the mutual similarity of reactor physics experiments and with respect to the target reactor system, as well as of the solution quality diagnosis methods (statistical tests, similarity coefficients, Cook's distance, calculation of the adjustment potential and motive force indicators, verification of biases obtained for being physical, etc.) (NEA/NSC/R(2016)6 2017).

Since the ONIX supports algorithms for constrained nonlinear multi-parameter optimization, this makes it possible to solve the problem of determining the required accuracies of neutron data which provide for the target accuracies of calculating the neutronics characteristics of reactor and fuel cycle systems. The standard mathematical formulation for the given problem (Usachev and Bobkov 1980) suggests that such nuclear data uncertainty values are searched for (uncertainty means a standard deviation, that is the root of variance) so that the uncertainty of the reactor functional due to nuclear data, R, estimated on their basis, does not exceed the target uncertainty, d_{tr} (variance), that is $d_R(d_i) \le d_{tr}$ (e.g., for a fast reactor's k_{eff}, the recent requirements (Castelluccio et al. 2021;

Cabellos 2021) to the prediction accuracy are in a range of 0.2 to 0.3%). The problem of determining the required accuracies of neutron constants is reduced to minimizing the so-called functional of 'costs', F, for obtaining information on each neutron constant. The costs of achieving accuracy, d_i, are commonly believed to be the product of the cost, λ_i, of obtaining a unit of information by the statistical neutron constant weight equal to $1/d_i$. The uncertainty of the reactor functional due to nuclear data, R, is determined from formula (Usachev and Bobkov 1980):

$$d_R = \mathbf{S}^{\mathrm{T}}\mathbf{M}_{\sigma}\mathbf{S},$$

where $S_i = \partial R / \partial \sigma_i$ are components of the vector of sensitivity coefficients for the calculated value of the reactor parameter to the i^{th} nuclear constant, and $\mathbf{M}_{\sigma}$ is the covariance matrix of nuclear data. The optimization problem for defining the requirements to the accuracies of neutron constants can be formulated as follows:

$$\begin{cases} F = \sum_i \lambda_i / d_i \to \min, \\ d_R = \mathbf{d}^{\mathrm{T}}\mathbf{S}_{\mathrm{D}}{}^{\mathrm{T}} C_{\sigma} \mathbf{S}_{\mathrm{D}}\mathbf{d} \le d_{tr}, \\ d_i \le d_{i,0} \ (i = 1, \ \ldots, \ N), \end{cases} \quad (2)$$

where $\mathbf{d} = \{d_i^{1/2}\}$ is the vector of nuclear constants uncertainties (standard deviation), $d_{i,0}$ is current constants uncertainties, $\mathbf{S}_{\mathrm{D}}$ is the diagonal matrix of sensitivity coefficients ($\mathbf{S}_{\mathrm{D}ii} = S_i$ for $i = j$ and $\mathbf{S}_{\mathrm{D}ij} = 0$ for $i \neq j$), and $\mathbf{C}_{\sigma}$ is the correlation matrix of neutron constants.

The ONIX calculations of the tests from the OECD Nuclear Energy Agency (NEA) developed for the cross verification of codes for analyzing uncertainties for reactor applications (Assessment of Existing Nuclear Data Adjustment Methodologies 2011), as well as the comparison with the results of calculations from other authors obtained using functionally similar software tools have demonstrated that the ONIX-supported procedures and algorithms are correct (specifically, the results obtained are identical for similar model assumptions and initial data).

The ONIX computation module has been developed using the Python programming language. To make it easier for users to operate the ONIX code, the module for the initial data preparation and post-processing of calculations results, has been developed with the use of the MS Excel Visual Basic for Applications (VBA) spreadsheet embedded language. Functionally limited educational versions of the ONIX code have also been developed in the MathCAD computerized algebra system.

Examples of the ONIX application

Defining requirements to the accuracy of neutron data that support the target accuracy of predicting stationary neutronics characteristics

The first example of the ONIX application is problem solving for defining requirements to the accuracy of neutron data that support the target accuracy of prediction for criticality of a lead-cooled fast reactor. The essence of the problem is that in conditions of high requirements to the accuracy of predicting the performance of innovative reactor plants (e.g., the prediction accuracy for k_{eff} needs to be $\delta k_{\mathrm{eff}} \le 0.3 - 0.2\%$ with the initial nuclear data uncertainty being $\delta k_{\mathrm{eff}} \ge 1\%$), one shall formulate requirements to the accuracy of neutron data that will make it possible to achieve the target accuracy of calculation for parameters of the facility under design. The results of such analysis are used at the OECD NEA to generate the list of high-priority requests (HPRL) for updated nuclear data.

Fig. 1 presents the results of solving the problem in question using the ONIX code assuming that neutron constants are expected to ensure the target accuracy of the k_{eff} calculation for a lead-cooled fast reactor model at a level of not more than 0.2%. The figure also presents the results of similar estimates from OECD NEA experts (Cabellos 2021; Castelluccio et al. 2021). Despite the fact that OECD NEA studies used the implementation of nonlinear optimization methods that are different from that used in the ONIX code, and the initial uncertainty values for neutron cross-sections (solid lines in the diagrams) were determined based on non-Russian evaluated nuclear data libraries, the results (dotted and dashed lines) have close trends on the whole and are practically identical in the fast reactor significant region of energies (1 keV to 1 MeV) (the ONIX calculations used the Russian evaluated nuclear data library, BROND 3.1, with 28 energy groups covariances, and the ENDF/B-VIII.0 library was used in Cabellos 2021 with covariances represented in seven energy groups).

The results obtained demonstrate that achieving the target accuracy of k_{eff} at a level of 0.2% without taking into account the integral experiments requires the uncertainties of neutron cross-sections to be reduced substantially (by 7 to 10 times), which is not always feasible through a multitude of differential measurements, primarily because the current experimental techniques lack the required precision.

Estimating the uncertainties associated with neutron data for target neutron multiplying systems taking into account integral measurement results

The second examples of the ONIX application is prediction of performance for neutron multiplying systems based on information on criticality measurements undertaken in critical assembly experiments. As the example for demonstration, the OECD NEA's test for critical safety of MOX fuel systems was considered (Andrianova et al. 2018; Carmouz et al. 2017) which has been proposed for testing national codes and neutron constants used to justify critical safety for reactor and fuel cycle systems. This test considers 15 different target systems which simulate the closed fuel cycle components. There were 12 informative BFS-based critical experiments selected to implement the reactor physics experimental data assimilation procedure (ICSBEP 2021).

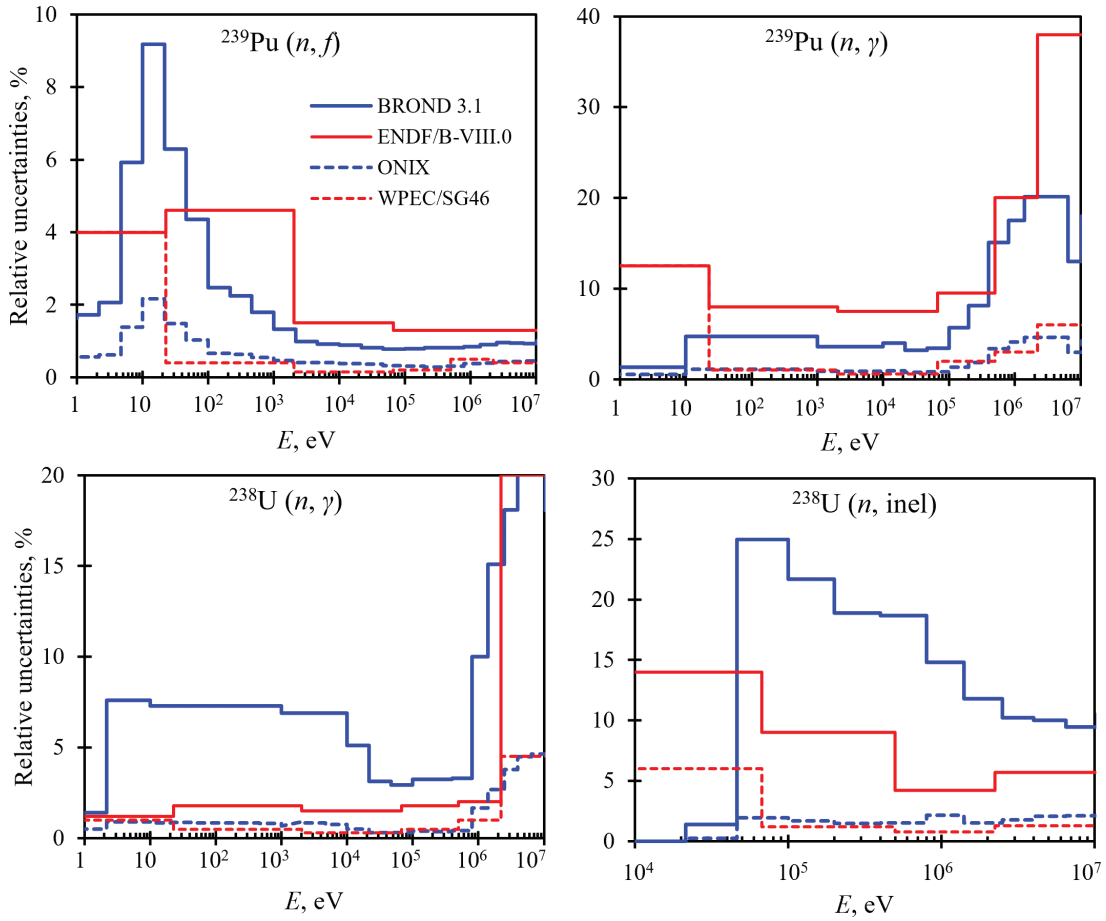

Figure 1. Relative uncertainties of important neutron reactions defining the k_{eff} uncertainty for a lead-cooled fast-reactor model due to nuclear data uncertainties (solid lines – uncertainties achieved, dashed and dotted lines – uncertainties required).

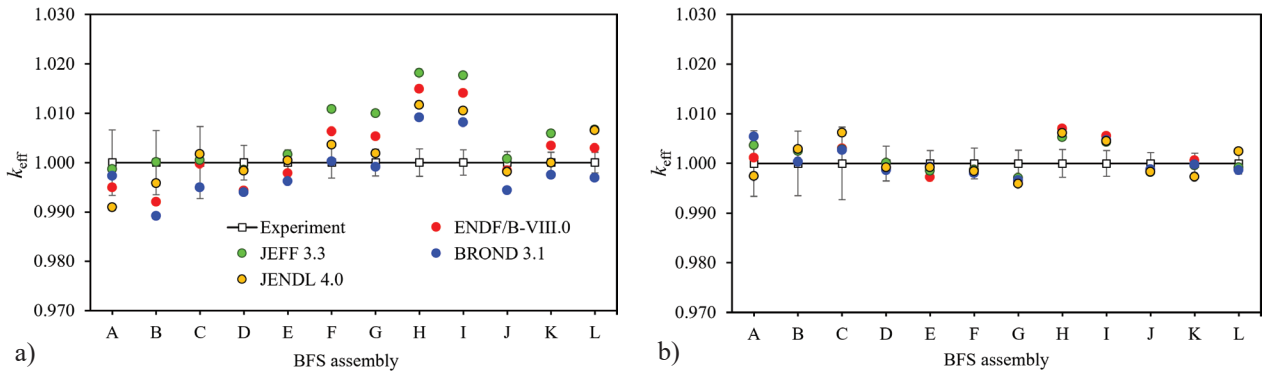

Figure 2. Calculation and experimental discrepancies in k_{eff}: prior to (a) and after (b) the neutron data adjustment. Letter designations for BFS assemblies: A – BFS-35-1; B – BFS-38-2; C – BFS-42; D – BFS-97-1; E – BFS-97-2; F – BFS-97-3; G – BFS-97-4; H – BFS-99-1; I – BFS-99-2; J – BFS-101-1; K – BFS-101-1; L – BFS-101-3.

The results of the ONIX application for solving the problem at hand using different evaluated neutron data sets are presented in Fig. 2. In particular, the figure demonstrates how adjusted neutron constants within the limits of their respective uncertainties allow reducing the calculation and experimental discrepancies for the considered set of critical experiments. As the result of the neutron data corrections based on the integral measurement data, the uncertainty of the target system calculation due to the nuclear data uncertainty is reduced (Fig. 3). It should be noted that different evaluated neutron data libraries become indiscernible in terms of quality after the adjustment: they ensure, on the average, similar calculation and experimental discrepancies (for the given set of reactor physics experiments).

Adjustment of uncertainties associated with nuclear data and technological parameters in post-irradiation experiments

The third example of the ONIX code application demonstrates joint adjustment of neutron constants and

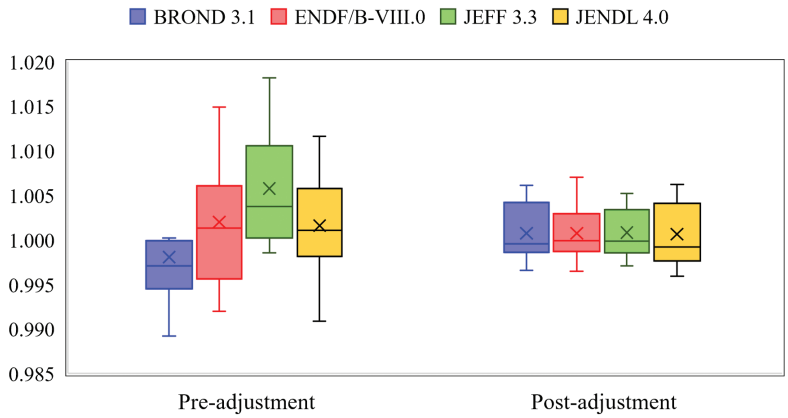

Figure 3. A priory and a posteriori k_{eff} uncertainties for the target system (for the case with a 30% content of plutonium in MOX fuel and a plutonium vector of 96, 4, 0, 0% for ^{239,240,241,242}Pu respectively): crosses – mean value, line inside rectangular boxes – median, rectangular box boundaries – 25 and 75% percentile, whiskers – minimum and maximum values.

technological parameters as applied to nuclide kinetics modeling problems. Cases may occur in developing benchmark models of post-irradiation experiments when the discrepancies between calculated and experimental values cannot be eliminated by adjusting only neutron data within the limits of their measurement uncertainties. In such cases, calculation and experimental discrepancies may be caused by other factors (e.g., by an inadequate calculation model, high uncertainties in technological parameters, etc.), so minimizing these discrepancies exclusively by adjusting neutron data may lead to nonphysical results. In cases when the reliability of experimental data is undisputable, it is possible to adjust the calculation model of experiments by adjusting as well the technological parameters in the limits of their respective uncertainties.

Technological parameters (sizes of structural elements, nuclear concentrations, temperatures of materials, etc.) define the conditions for a particular measurement. Apart from the above parameters, essential for nuclide kinetics problems are fuel irradiation modes (irradiation and cooling times, thermal power, etc.). As a rule, specific to this class of problems is major effect of the technological parameter uncertainties (primarily for the initial composition, Table 2) on the uncertainty of determining the irradiated sample composition. In such situations, the calculated uncertainty component defined by the technological parameter uncertainties (Table 3, column 2) turns out to be comparable or even higher in terms of the nuclear data component value (Table 3, column 3), unlike stationary neutronics problems where the nuclear data component of the uncertainty may prevail.

In this case, combined adjustment of all input data (both technological parameters and neutron data) leads to these being updated (the isotopic composition is updated within the limits of the declared uncertainties), both uncertainty components reduced, and the calculated and experimental values converging.

Table 3 presents the adjustment results for technological parameters (nuclear concentrations of the initial fuel composition, one-group neutron flux, cooling time) and

Table 2. Uncertainties in one-group cross-sections and initial composition of irradiated sample

Nuclide	Uncertainties in one-group cross-sections (BROND 3.1), %		Uncertainties in initial composition, %
	(n, fis)	(n, γ)	
^{234}U	1.8	25.1	33
^{235}U	0.6	5.5	3.3
^{236}U	0.6	3.2	-
^{238}U	0.7	4.5	0.04
^{238}Pu	2.2	26.5	50
^{239}Pu	0.7	4.3	0.2
^{240}Pu	1.4	5.1	4.5
^{241}Pu	3.2	6.6	33
^{242}Pu	2.5	7.6	100
^{241}Am	1.0	7.4	25
^{242m}Am	2.8	17.4	-
^{243}Am	3.0	3.7	-
^{242}Cm	12.4	19.2	-
^{243}Cm	9.6	17.7	-
^{244}Cm	4.2	17.8	-

Table 3. The irradiated fuel composition calculation uncertainties due to technological parameters (T) and neutron data (N) uncertainties

Nuclide	Irradiated fuel composition uncertainties, %			
	A priory		A posteriori	
	T	N	T	N
^{234}U	30	2.2	2.8	1.8
^{235}U	3.0	0.5	1.0	0.4
^{236}U	2.9	5.2	0.9	3.7
^{238}U	0.04	0.2	0.04	0.04
^{238}Pu	14	3.1	2.7	2.0
^{239}Pu	0.13	1.2	0.13	0.2
^{240}Pu	1.8	2.7	1.5	1.5
^{241}Pu	3.9	4.8	2.9	2.5
^{242}Pu	29	4.8	3.7	2.9
^{241}Am	13	2.6	1.5	1.3
^{242m}Am	23	6.4	0.5	1.1
^{243}Am	47	7.6	5	3.7
^{242}Cm	22	6.2	0.5	0.9
^{243}Cm	24	20.0	0.6	2.7
^{244}Cm	57	7.9	6	4.3

neutron constants (one-group fission, capture, (n,2n) reaction neutron cross-sections, branching ratios, etc.) for updating the benchmark model of the experiment to examine irradiated samples of uranium-plutonium fuel in a fast reactor (Momotov et al. 2022). Adjustment of technological parameters using the authors modification of the ONIX-supported Lagrange indefinite multiplier method makes it possible to reduce the uncertainty component induced by technological parameters uncertainties by about a factor of 10. The algorithm used minimizes quadratic form (1) provided the experimental and calculated values are equal (**C**(**x**) = **E**). This suggests that the biases in the adjusted parameters shall not exceed the initial uncertainties of $|\mathbf{x} - \mathbf{x}_0| \leq \mathbf{d}_0^{1/2}$.

Conclusions

The application scope of the ONIX code is to adjust neutron constants and technological parameters for neutronics models based on the results of reactor physics experiments. The code can be used to update stationary and time-dependent neutronics models of nuclear reactors and fuel cycle facilities, benchmark models of reactor physics experiments, and estimate reactor characteristic uncertainties associated with nuclear data and technological parameters. It can also be used to determine the accuracy of predicting the neutronics performance of reactors and related fuel cycles. Additionally, the code allows for determining the required neutron data uncertainties needed to achieve the target accuracy of neutronics performance prediction. The implemented method for constrained multi-parameter nonlinear optimization significantly expands the application scope of classical approaches to neutronics data assimilation, such as maximum likelihood and generalized least squares methods. This implementation is reduced to the latter when defining the problem for searching for the unconstrained minimum. The proposed procedure allows for solving inverse problems on specifying requirements for neutron data accuracies and determining the optimal set of additional differential and reactor physics experiments necessary to achieve the target accuracy in predicting the neutronics performance of reactor and fuel cycle systems under design.

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