





**Research Article** 

# Nuclear energy system modelling application package: functional overview and examples<sup>\*</sup>

Andrei A. Andrianov<sup>1</sup>, Ilya S. Kuptsov<sup>1</sup>, Tatiana A. Osipova<sup>1</sup>, Anastasia A. Spiridonova<sup>1</sup>, Olga N. Andrianova<sup>1</sup>, Tatiana V. Utianskaya<sup>1</sup>

1 IATE, NRNU MEPHI, 1 Studgorodok, 249039 Obninsk, Kaluga Reg., Russia

Corresponding author: Andrei A. Andrianov (andreyandrianov@yandex.ru)

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# Abstract

The paper provides a brief description of the functionality of the nuclear energy system modelling application package (NESAPP), including a list of modelling objects, key assumptions and areas of application. NESAPP consists of the following main modules: NUDAPS (a module for calculating thermal neutron cross-sections, resonance integrals and one-group neutron cross-sections, and associated uncertainties), NUCLEX (a module for calculating the evolution of the nuclide composition and characteristics of nuclear fuel in reactors and at the nuclear fuel cycle front-end and back-end steps), NUCAB (a module for adjusting isotopic composition and blending), FANES (a module for analysing material flows and integrating data in nuclear energy evolution scenarios), ECNES (a module for assessing economic performance metrics for the nuclear energy evolution scenarios). Each of the modules is a calculation tool that can be used as independent or integrated into the software for technical and economic modelling of nuclear energy systems. Various calculation models are implemented in the modules, allowing users to evaluate the methodological component of the calculation uncertainty in scenario modelling studies and the functionality for assessing the impact of initial data uncertainties on the resulting indicators. The authors also provide some examples of applying NESAPP.

# Keywords

Nuclear energy system, nuclear fuel cycle, technical and economic modelling, scenario analysis, material flow analysis, economic analysis

# Introduction

Software tools for conducting technical and economic modelling of nuclear energy systems (NES) and scenario (system) studies in the field of the nuclear fuel cycle (NFC) make it possible to estimate the change in time of the volume of material flows along the NFC stages, the need for various NFC services and goods, indicators of efficiency and competitiveness of the NES option, taking into account various external and internal factors (the NES refers to the NPP system and the NFC enterprises associated with this system). The corresponding computational models can be constructed at the level of an energy company, a country, a region, or even the whole world and assume a significant representation of the key processing stages of the associated NFC and physical processes that

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occur with nuclear materials during their circulation in the NES fuel cycle (Silvennoinen 1982, Klimenko 2010, Muravev 2019, Brown et al. 2016, Andrianov et al. 2020).

Such software tools are used for a comprehensive analysis and feasibility study of possible NES deployment options, optimisation of NES options in terms of a set of performance indicators (taking into account resource and infrastructure constraints), comparison of alternative NES options, NFC organization approaches, approaches to radioactive waste management and selection of the most acceptable ones under given conditions, studies of the impact of technological improvements and new developments on the NES performance indicators.

The corresponding calculation tools integrate submodels of various levels: physical models that make it possible to assess changes in the nuclide composition and characteristics of nuclear fuel in reactors and in the different NFC steps during the NES evolution; models of the dynamics of the movement of nuclear materials in the NFC; models for assessing NES economic efficiency indicators; and market models of NPPs, NFC goods and services. The software tools are used in conjunction with specialised databases containing information on the current state and prehistory of the NES development at the appropriate level (global, regional, country, corporate), as well as the technical and economic parameters of operating and planned reactor plants and NFC facilities.

Despite the existing arsenal of models, approaches, and software tools for systematic studies of the prospects for the development of nuclear energy, systematic work is currently underway on further upgrading and improving them in order to provide the possibility, on their basis, of developing technical and economic NES models with increased accuracy (correct modelling of material flows in the NFC, taking into account nuclide evolution, refinement of estimates of economic indicators, etc.), as well as on translating into computer codes the optimisation and prioritisation mechanisms for overcoming technological forks, the functionality of sensitivity and uncertainty analysis, exploratory data analysis, aggregation of system-wide indicators and multi-criteria comparative evaluation (Andrianov et al. 2020). One of such developments is the nuclear energy system modelling application package (NESAPP): the description of its functionality (including a list of modelling objects, key assumptions, application areas) is given in this paper. It should be noted that the authors do not provide a description or analysis of the advantages and disadvantages of other programmes as this is not within the scope of the current study.

# Brief description of NESAPP

The NESAPP software modules are designed for calculation support of studies in the field of nuclear energy planning, scenario modelling of the nuclear energy development, system-level assessment of reactor and NFC technologies both as independent calculation tools and as part of applied software packages for technical and economic modelling of nuclear energy systems. On the basis of the software modules, it is possible to construct complex calculation models for assessing material flows and needs for NFC services (needs for natural uranium, services for uranium conversion and enrichment, fresh fuel fabrication, SNF storage and reprocessing, etc.) and economic performance metrics of NES development scenarios. The main software modules include:

- NUDAPS (Nuclear Data Processing Spreadsheets): preparation of one-group neutron cross-sections averaged over standardised and (or) user-specified neutron spectra;
- NUCLEX (Nuclide Evolution Explorer): calculation of the evolution of the nuclide composition and characteristics of nuclear fuel in reactors and at the main NFC front-end and back-end steps;
- NUCAB (Nuclide Composition Adjustment and Blending Tool): correction of the nuclide composition of the fuel and neutron flux; if necessary, the modelling of the reactor operation on the new isotopic composition of fresh nuclear fuel;
- FANES (Material Flow Analysis Data Integrator for Nuclear Energy System): assessment of material flows and needs for NFC goods and services in nuclear energy development scenarios;
- ECNES (Economic Assessment Tool for Nuclear Energy System): assessment of economic performance metrics for nuclear energy development scenarios.

The general flow chart of NESAPP is shown in Fig. 1. It should be emphasized that the current release of NE-SAPP implements the traditional practices in this subject area for conducting system-wide economic assessments of nuclear energy systems, which are also used in similar foreign and Russian software tools (Andrianov et al. 2020), which, however, do not imply modelling the organisation of the operation of the entire energy system (consideration of all types of generation, consumers, technological restrictions, net power flows, operation of the WMEP, price zones, tariffs, etc.). Also, at the current stage, NESAPP does not assess the needs for personnel of NPPs and NFC facilities.

Characteristic features of NESAPP are the modular principle of software organization, the autonomy of the modules, the multiplicity of implemented calculation models in each module, the assessment of the uncertainties of the calculation functionals in accordance with the uncertainty of the initial data. In addition, NESAPP is accompanied by a database of typical reactor characteristics, an atlas of one-group neutron cross-sections for various neutron spectra (for nuclide evolution modelling), and a database with data on neutron spectra. The user can form sets of initial data in accordance with the task under consideration. The user is responsible for generating



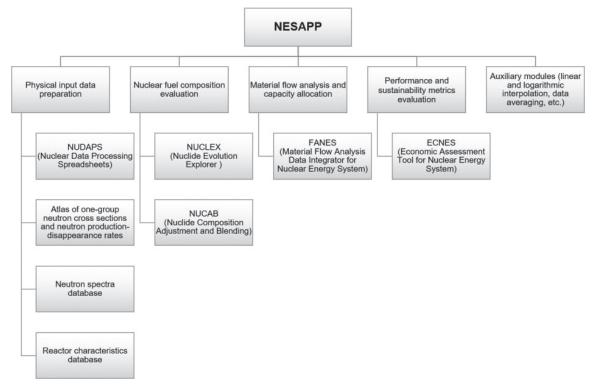


Figure 1. General flow chart of NESAPP.

a set of initial data for conducting economic assessments according to the study context and model assumptions implemented in the ECNES module. The assumptions of the calculation models implemented in the NESAPP software modules are specified in the user instructions (Andrianov et al. 2021a, 2021b, Andrianov and Andrianova 2021a, 2021b, Andrianov 2021). The implemented model assumptions are typical of software tools for technical and economic modelling of nuclear energy systems (Table 1).

The NESAPP modules are created using the built-in spreadsheet language – MS Excel Visual Basic for Applications (VBA) (basic option) (Software for Working with MS Excel Spreadsheets).

There are also versions of NESAPP modules developed using the Python programming language, the MathCAD computer algebra system (Engineering Mathematical Software Mathcad), and the Stella Architect system dynamics modelling environment (Stella Architect Modelling Tool) using built-in programming languages. Accordingly, to work with NESAPP, the Microsoft Office application package is required. If the versions of the software modules for MathCAD and Stella Architect are used, the appropriate modelling environments must be available.

Work with NESAPP is carried out through the standard MS Excel interface. If the versions of the software modules for MathCAD and Stella Architect are used, the appropriate engineering graphical interfaces are available. All the programme modules are alienable; the need for author's support is determined by the user's qualifications.

The potential user of NESAPP is assumed to have knowledge of the basics of nuclear engineering, the principles of nuclear energy planning and the economics of nuclear energy. The computation time using the models developed with NESAPP is determined by their complexity and can range from a few seconds to several hours.

### Verification of NESAPP

The software modules were verified using software tools similar in functionality (Modelling Nuclear Energy Systems with MESSAGE, INPRO Methodology, Nuclear Fuel Cycle Simulation System). Identical results were obtained for similar model assumptions and initial data.

NESAPP was comprehensively tested using test problems developed for the purpose of cross-verification of Russian software tools for technical and economic modelling of nuclear energy systems. The cross-verification was carried out in the format of voluntary (initiative) activity in the period of 2020-2021 (Altynnikova et al. 2021). In accordance with the technical and economic data given in the descriptions of the test problems as well as taking into account the assumptions regarding the management of SNF and secondary fissile materials, NESAPP was used to develop calculation models to simulate nuclear material flows, the structure and dynamics of changes in the installed capacity of the considered NES options. The models make it possible to calculate material indicators, including material flows and needs for NFC goods and services as well as economic indicators. The results of calculations performed using NESAPP are consistent with the calculations performed by other participants in cross-verification (the observed discrepancies in the calculations are explained by the model features of the software tools involved).

Table 1. Assumptions and	Implemented Calculation	Models in the NESAPP Modules

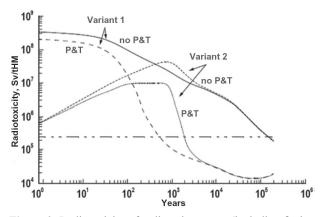
Module	Purpose	Initial data	Assumptions / functional
NUDAPS	tron cross-sections, various functionals, which are linear combinations, products and ratios of one-group neutron cross-sections and their uncer- tainties	matrices, neutron spectrum (these data are placed in a specialised database of evaluated neutron data of actinide nuclei)	and BOXER formats (for covariance matrices), a set of standardized neutron spectra (fission, Maxwell, Fermi, etc.) and neutron spectra characteristic of various types of power reactors (the spectra can be specified in both analytical and tabular forms).
NUCLEX	Calculation of nuclide com- position evolution (mass and concentration), activity, radio- toxicity, heat release, neutron and gamma sources of nuclear fuel	Initial isotopic composition of the fuel, one-group neutron fluxes and neutron cross-sections, both determined at vari- ous stages of fuel irradiation in the reac- tor and one-group flux and cross-sections averaged over the entire irradiation cycle and constant in time, specific power den- sity, nuclear fuel burnup	Basic set of actinide nuclei: <sup>234</sup> U, <sup>235</sup> U, <sup>236</sup> U, <sup>238</sup> U, <sup>237</sup> Np, <sup>238</sup> Pu, <sup>239</sup> Pu, <sup>240</sup> Pu, <sup>241</sup> Pu, <sup>242</sup> Pu, <sup>241</sup> Am, <sup>242</sup> Am, <sup>243</sup> Am, <sup>242</sup> Cm, <sup>243</sup> Cm, <sup>244</sup> Cm, <sup>245</sup> Cm, <sup>246</sup> Cm, <sup>247</sup> Cm, <sup>248</sup> Cm. Basic set of fission and activation products: <sup>3</sup> H, <sup>14</sup> C, <sup>36</sup> Cl, <sup>54</sup> Mn, <sup>55</sup> Fe, <sup>60</sup> Co, <sup>59</sup> Ni, <sup>63</sup> Ni, <sup>79</sup> Se, <sup>85</sup> Kr, <sup>87</sup> Rb, <sup>90</sup> Sr, <sup>93</sup> Mo, <sup>94</sup> Nb, <sup>93</sup> Zr, <sup>98</sup> Tc, <sup>99</sup> Tc, <sup>102</sup> Rh, <sup>106</sup> Ru, <sup>107</sup> Pd, <sup>110m</sup> Ag, <sup>113m</sup> Cd, <sup>121m</sup> Sn, <sup>125</sup> Sb, <sup>126</sup> Sn, <sup>125m</sup> Te, <sup>127m</sup> Te, <sup>126</sup> Sn, <sup>132</sup> Eu, <sup>154</sup> Eu, <sup>155</sup> Eu, <sup>166m</sup> Ho. Output data (masses and concentrations of the main actinides, fission products, radioactivity, decay heat, radiotoxicity, neutron and gamma radiation) are given for the end of the irradiation cycle, after cooling, for the 100th, 1000th and 10000th years. The functionality for estimating the nuclear data and technological uncertainty of the design characteristics is implemented.
NUCAB	uncertainties of the corrections	Fuel isotope composition (design and ac- tual), one-group neutron cross-sections, covariance matrices and neutron flux	Various methods for estimating the enrichment and total neu- tron flux corrections and their uncertainties are implemented in order to select the most appropriate method for its sub- sequent implementation. The uncertainties of the corrections associated with the initial neutron data are estimated.
FANES	and needs for NFC goods and	missioning of power units, parameters of fuel use and SNF/RW production, isotope composition of fresh and spent fuel, char- acteristics of the strategy for handling SNF/RW, fissile materials, principles of	stages of the NFC and in SNF storage facilities, set priorities
ECNES		Dynamics of commissioning and decom- missioning of power units, technical and economic parameters of power units, material flows and needs for NFC goods and services (needs for natural uranium, uranium conversion and enrichment ser- vices, fresh fuel fabrication, SNF storage and processing, etc.), cost data on con- struction, operation and decommission- ing of power units, NFC goods and ser- vices, discount rate, electricity tariff	ond degree polynomial, arbitrary distribution), adjust capital costs for units that remain in operation beyond the forecast

# Some examples of NESAPP applications

The NESAPP software modules have been used since 2008 for calculation support of studies in the field of nuclear energy planning, scenario modelling of nuclear energy development, assessment of nuclear energy technologies and NFC technologies at the Obninsk Institute for Nuclear Power Engineering of the National Research Nuclear University MEPhI as part of various initiative and contractual research projects (Andrianov et al. 2014, 2022, Andrianov and Kovganko 2020). Below are some examples of actual applications of NE-SAPP (it should be emphasized that all the examples are illustrative and given only to show the workability of the created toolkit).

### Modelling of partitioning and transmutation scenarios taking into account the generation of radionuclides over time

Using NESAPP, a simulation of scenarios for the partitioning and transmutation of RW generated during the operation of a hypothetical NES with thermal reactors for 1000 years was carried out under two assumptions: the simultaneous appearance of the entire volume of RW (Option 1) and the gradual production of RW in accordance with the scenario of the NES operation (Option 2) (Andrianov et al. 2014). In both considered scenarios, the same assumptions are made regarding the integral amount of natural uranium required for the fabrication of fresh fuel and the generated RW undergoing transmutation (plutonium and minor actinides are burned in accelerator-driven systems, the integral efficiency of partitioning and transmutation process in both scenarios is the same (the integral efficiency of partitioning and transmutation process  $\varepsilon_{pT} = \varepsilon_p \varepsilon_T / (1 - (1 - \varepsilon_T) \cdot \varepsilon_p)$ , where  $\varepsilon_{r}$  is the burnup depth per irradiation cycle and  $\varepsilon_{p}$  is the individual partitioning efficiency). As a reference level, which makes it possible to compare the effectiveness of the partitioning and transmutation strategy by estimating the time it takes for the selected indicator to reach a given level, the radiotoxicity (during the oral intake of radionuclides into the body) of natural uranium is used, which is required for the fabrication of fresh fuel in order to ensure the NES operation throughout the entire life cycle.



**Figure 2.** Radiotoxicity of radioactive waste (including fission products, activation products, actinides) upon oral intake of radionuclides into the body for the considered NES scenario.

It is shown that, under comparable conditions, Option 1 (without taking into account the RW production over time) gives an underestimated time for reaching the given reference level by the selected indicator compared to Option 2 (taking into account the RW accumulation over time) (Fig. 2). However, if the duration of the NES operation does not exceed 300 years, then this difference can be neglected (the bias in the time needed to reach the reference level will not exceed 200 years). In the scenarios where the NES operation is assumed to be over 300 years, the assumption not to take into account the RW generation over time will be an incorrect, since the bias in determining the time to reach the reference level will significantly exceed 200 years. In general, the estimates show that the longer the NES operates, the less pronounced is the effect of RW transmutation.

#### Modelling of scenarios for the development of the russian two-component NES with thermal and fast sodium reactors

NESAPP was used in modelling scenarios for the development of the Russian two-component NES with thermal and fast sodium reactors (Andrianov et al. 2022). The following scenarios were considered in the NES structure in 2100:

- VVER(100%): share of VVER-TOI = 100%;
- VVERmox(10%): shares of VVER-TOI, VVER-TOI MOX = 90 and 10%;
- VVERmox(30%): shares of VVER-TOI, VVER-TOI MOX = 70 and 30%;
- VVERmox(50%): shares of VVER-TOI, VVER-TOI MOX = 50 and 50%;
- BN(20%): shares of VVER-TOI, BN = 80 and 20%;
- BN(50%): shares of VVER-TOI, BN = 50 and 50%;
- BN(90%): shares of VVER-TOI, BN = 10 and 90%;
- VVERmox(10%) BN(20%): shares of VVER-TOI, VVER-TOI MOX, BN = 70, 10 and 20%;
- VVERmox(50%) BN(20%): shares of VVER-TOI, VVER-TOI MOX, BN = 30, 50 and 20%;
- VVERmox(10%) BN(50%): shares of VVER-TOI, VVER-TOI MOX, BN = 40, 10 and 50%.

It is shown that, when the assessment of NES deployment scenarios is based on exclusively of material and economic indicators, the involvement of MOX-fuelled thermal reactors in the two-component NES leads to a decrease in the attractiveness of the corresponding scenario compared to scenarios without MOX fuel in thermal reactors (Table 2). It should be noted that the issue of using plutonium in thermal reactors requires a detailed study due to the lack of undeniable arguments indicating the feasibility of implementing this option: it may make sense to consider other points that can make this technological option expedient (providing a technology reference for export, the need to burn surplus plutonium, etc.).

# Estimation of the levelised unit energy cost at NPPs with different types of nuclear reactors

NESAPP was used to estimate the levelised unit energy cost (LUEC) at NPPs with different types of nuclear reactors, with account taken of the uncertainty in the cost data for the construction and operation of reactor plants as well as for the NFC goods and services (Table 3) (Andrianov and Kovganko 2020).

Three types of thermal reactors (LWR, HWR and ALWR) operating in an once-through NFC and four variants of fast reactors (FR-1, FR-2, AFR and FR-U) operating in a closed uranium-plutonium NFC were considered (data for the relevant technologies were taken from the international IAEA INPRO GAINS project, cost data were from a report prepared as part of one of the studies in the interests of the US Department of Energy (Andrianov and Kovganko 2020)).

Scenario (technology share in 2100 is in parentheses) / indicator	Cumulative uranium consumption, kt	Cumulative needs for uranium enrichment services, 10 <sup>6</sup> SWU	Cumulative needs for spent fuel reprocessing services, kt h.m.	Amount of SNF in 2100, kt h.m.	Amount of RW in 2100, kt h.m.	Amount of plutonium in the NFC in 2100, kt	Amount of depleted uranium in 2100, kt	LUEC, mills/kWh
VVER(100%)	787.65	666.75	0	126.98	0	1.09	1669.03	29.48
VVERmox(10%)	782.92	662.72	27.36	106.12	26.92	0.84	1658.34	29.89
VVERmox(30%)	776.18	656.97	71.81	69.11	70.76	0.54	1644.80	30.40
VVERmox(50%)	772.07	653.46	92.71	51.06	91.42	0.41	1638.11	30.57
BN(20%):	658.10	556.25	12.15	111.54	10.96	1.02	1544.24	29.53
BN(50%):	492.27	414.81	41.77	77.70	38.93	0.91	1384.26	30.22
BN(90%):	284.97	237.99	100.28	13.96	95.37	0.76	1184.07	31.09
VVERmox(10%) BN(20%)	651.51	550.63	346.08	81.58	46.76	0.77	1531.93	30.29
VVERmox(50%) BN(20%)	640.97	541.64	126.27	14.46	123.68	0.34	1511.78	31.57
VVERmox(10%) BN(50%)	470.99	396.66	79.63	44.59	76.26	0.65	1359.36	31.70

Table 2. Key Performance Indicators of the 10 NES Development Scenarios

- LWR is a PWR type reactor with a burnup of 45 GW·day/t h.m., fuel enrichment of 4%, a specific core energy density of 38.5 MW/t, and a capacity factor of 85%.
- ALWR is an advanced LWR with higher fuel burnup; compared to LWR, equilibrium fuel loading in ALWR is 30% less than in LWR, initial fuel enrichment is 3.4%, equilibrium fuel enrichment is 4.95%.
- HWR is a pressurised heavy water nuclear reactor with a burnup of 7 GW·day/t h.m., fuel based on natural uranium, a specific power density of 24.0 MW/t, and a capacity factor of 85%.
- FR-1 is a sodium-cooled fast reactor with a breeding factor close to unity and an average fuel burnup (core and blankets) of about 38 GW·day/t h.m.
- FR-2 is a prototype sodium-cooled fast breeder reactor with an average breeding factor of 1.16 and an average fuel burnup (core and blankets) of about 31 GW·day/t h.m.
- AFR is a commercial sodium-cooled fast reactor with an average breeding factor of 1.2 and an average (core and blankets) fuel burnup of 54 GW·day/t h.m. Unlike FR-1 and FR-2, fresh AFR fuel contains about 1% minor actinides (MA).
- FR-U is a lead-cooled fast reactor that uses enriched uranium fuel (enrichment of about 15% in <sup>235</sup>U) for initial core loading and first refuelling; subsequent SNF reprocessing and the use of secondary nuclear fuel (Pu + U + MA) are assumed. The blanket is not provided. The breeding factor is 1.05, fuel burnup is about 72.8 GW·day/t h.m.

Based on the results of assessing the levelised unit energy cost and with account taken of the uncertainty in its values due to the spread in cost data, it can be concluded that it is impossible to make an unambiguous judgment about the greatest attractiveness of a particular concept of fast reactors, relying only on the analysis of the levelised unit energy cost, and it is also incorrect to Table 3. LUEC and its components

Type of NES	LUEC and its components, mills/kW·h				
	LUAC	LUOM	LUFC	LUEC	
LWR*	37.6±9.3	12.2±1.2	8.9±2.3	58.7±9.6	
LWR**	$37.6 \pm 9.5$	$12.2 \pm 1.2$	9.9±2.3	$59.8 \pm 9.8$	
HWR*	36.2±9.1	$12.2 \pm 1.3$	$10.6 \pm 2.0$	59.2±9.3	
HWR**	36.2±9.1	$12.2 \pm 1.2$	17.6±3.2	$65.8 \pm 9.8$	
ALWR*	$35.4 \pm 8.8$	$11.6 \pm 1.2$	6.7±1.5	$53.8 \pm 9.0$	
ALWR**	$35.3 \pm 8.7$	$11.6 \pm 1.2$	7.5±1.5	$54.5 \pm 9.1$	
FR-1	$40.2{\pm}12.0$	$12.5 \pm 1.2$	13.5±2.4	66.2±12.4	
FR-2	40.0±12.1	$12.5 \pm 1.2$	14.2±2.4	67.3±12.4	
AFR	40.4±12.1	$12.6 \pm 1.2$	$8.9 \pm 1.5$	61.4±12.1	
FR-U	40.4±12.0	12.6±1.2	12.9±2.0	65.7±12.2	

\* — SNF storage in a centralised storage facility outside the reactor building throughout the entire life cycle, \*\* — final SNF disposal in deep geological formations after 5 years of cooling LUAC is the levelized unit life cycle amortization cost; LUOM is the levelised unit life cycle operation and maintenance cost; LUFC is the levelized unit life cycle fuel cost.

make categorical statements about the lower economic efficiency and competitiveness of fast reactors compared to thermal reactors.

# Conclusion

The nuclear energy system modelling application package (NESAPP) is intended for calculation support of scenario studies and technical and economic modelling of nuclear energy systems. The performed verification and cross-verification calculations using similar in functionality software tools and analogous model assumptions have demonstrated the correctness of the methods and algorithms implemented in the NESAPP. The experience of using NESAPP allows us to conclude that the developed toolkit is an effective means of supporting studies in the field of nuclear energy planning and scenario modelling, especially in the cases where it is necessary to assess the impact of uncertainties in the initial data and model assumptions on the calculation results.

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