

CONFERENCE PRE-PRINT

THE BENCHMARK DATABASE OF EXPERIMENTS, NUCLEAR, AND TECHNOLOGICAL DATA FOR HYBRID FUSION SYSTEMS WITH VARIOUS TYPES OF BLANKETS

M.N. SHLENSKII

NRC Kurchatov institute

Moscow, Russian Federation

Email: mike.shlenskii@gmail.com, yury.titarenko@itep.ru

S.A. BALYUK, V.F. BATYAEV, K.G. CHERNOV, V.M. CHERNOV, V.D. DAVIDENKO, D.N. DEMIDOV, A.V. GOLUBEVA, A.N. KIRSANOV, A.A. KOVALISHIN, B.V. KUTEEV, I.V. MEDNIKOV, A.M. OVCHARENKO, K.V. PAVLOV, A.P. PERSIANOVA, T.A. SHISHKOVA, A.B. SIVAK, P.A. SIVAK, M.L. SUBBOTIN, R.S. TIKHONOV, A.YU. TITARENKO, YU.E. TITARENKO, YA.O. ZARITSKY, V.M. ZHIVUN

NRC Kurchatov institute

Moscow, Russian Federation

Abstract

The article presents the results of developing databases intended to support the project on the design of a fusion neutron source carried out under the scientific supervision of the NRC “Kurchatov institute”. The work was conducted in three directions, each resulting in the development of an independent database: 1. Benchmark experiments for the verification of transport codes and evaluated nuclear data libraries used in blanket calculations for hybrid systems and in the assessment of activation of their structural and functional materials; 2. Evaluated nuclear data libraries (ENDF/B, ROSFOND, etc.), integrated into the VISTUD hardware-software system for their storage, processing, and visualization; 3. Properties of functional and structural materials intended for the design of hybrid facilities. The developed databases are planned to be integrated into a unified management system providing authorized user access with differentiated permissions, as well as prompt content updates by administrators.

1. INTRODUCTION

Fusion neutron sources (FNS) are considered one of the most promising approaches for the production of fissile nuclides required for nuclear power. Such facilities may also be employed for the transmutation of long-lived isotopes from spent nuclear fuel (SNF) of fission reactors, as well as for the production of isotopes used in various fields of medicine, science, and technology [1, 2]. The FNS concepts under development at the NRC “Kurchatov institute” are based on a tokamak-type magnetic confinement system for deuterium–tritium plasma, equipped with a blanket containing nuclear materials. The first stage towards the implementation of an industrial hybrid reactor is the development of an experimental prototype, FNS-1. At present, the FNS concept is also being considered for advancing the thorium–uranium nuclear fuel cycle.

In the design of an FNS, a key aspect is the simulation of neutron irradiation effects on the structural and functional materials of the facility. The results of simulations of neutron interactions with various materials, including fertile nuclear materials within the blanket, are determined by the evaluated nuclear data libraries employed [3]. Calculation practice demonstrates the necessity of conducting benchmark experiments for the verification of transport codes and evaluated nuclear data libraries applied in blanket calculations for hybrid systems and in the assessment of material activation.

Another critically important issue in FNS design is the selection of structural and functional materials, taking into account changes in their physicochemical properties during operation. For FNS, particular importance is attached to the limits of radiation-induced damage in materials, their adsorption properties with respect to hydrogen and helium, and activation characteristics. For instance, the proper selection of steel grade can reduce the residual induced activity by several times [4, 5].

Structuring of benchmark experimental data, results of their comparative analysis, material characteristics, and evaluated nuclear data library files within a management system will facilitate the efficient development of technical solutions in the design of FNS and provide all project participants with access to up-to-date information. Another important application of the developed databases is the possibility of referencing original experimental

data, the direct inclusion of which in scientific articles is often constrained by volume limitations. This, in turn, will allow other researchers to verify published results as well as their own transport codes and data libraries.

2. ABOUT DATABASES

2.1. Benchmark experiments database

The database was filled with results obtained both from benchmark experiments and from their numerical simulations. In the absence of high-intensity fusion neutron sources for conducting benchmark experiments aimed at verifying nuclear data, the following facilities were employed:

- the NG-24 neutron generator with a fusion-like spectrum and an intensity of 1×10^{11} n/s;
- the I-2 linear particle accelerator with a beryllium (Be) target irradiated by protons with an energy of 20.8 MeV and an intensity of 6×10^{11} proton/s.

A detailed description of the experimental setups and measurement techniques is given in [6, 7].

For the verification of computational results, each benchmark experiment included measurements of more than 800 threshold reaction rates, (n,2n), (n,p), (n,pn), (n, α), (n,n' γ), and (n, γ), on 17 samples of both natural and highly enriched isotopic compositions: $^{63}(99.5\%), ^{65}(99.7\%), \text{natCu}$, $^{\text{nat}}\text{Ni}$, $^{\text{nat}}\text{Zr}$, ^{27}Al , $^{\text{nat}}\text{Ti}$, ^{59}Co , $^{\text{nat}}\text{Mg}$, $^{\text{nat}}\text{Fe}$, $^{\text{nat}}\text{Cd}$, $^{\text{nat}}\text{In}$, $^{64}(99/4\%)\text{Zn}$, ^{197}Au , ^{93}Nb , ^{169}Tm , ^{232}Th . Reaction rates of residual nucleus production were measured by nondestructive gamma spectrometry.

Numerical simulations of reaction rates and neutron spectra were performed using various transport codes, including KIR, MCNP, SuperMC, and PHITS. The following evaluated nuclear data libraries were employed: JEFF-3.3, JENDL-4.0, ENDF/B-VIII.0, ROSFOND-2010, FENDL-3.0, TENDL-2019, IRDFF-II, and JENDL-5. Comparison of experimental and calculated data was carried out through statistical analysis of their ratios using three criteria (mean value and two variance estimators) [3]. The criteria were evaluated both for individual reactions and nuclides (averaged over libraries) and for each library (averaged over reactions and nuclides). These criteria serve to assess the predictive capability of the codes and to verify nuclear data libraries.

At present, the database contains data for micro-models of fusion blankets of various compositions [3, 6, 8]:

- the “pure” NG-24 spectrum (without a blanket);
- a molten salt blanket ($0.52\text{NaF} - 0.48\text{ZrF}_4$) with thermal and fast neutron spectra;
- solution-based blankets;
- experiments with a Be target irradiated by protons.

For each type of experiment, the database includes:

- a description of the experiment and the blanket geometry with the arrangement of irradiated samples;
- measurement results, including raw γ -spectra of the irradiated samples and their processed data;
- detector specifications and parameters of their absolute efficiency;
- simulation results obtained with different versions of transport codes and nuclear data libraries, provided in the form of input and output files;
- results of the comparison between experimental and calculated data for irradiated samples, presented as statistical factors.

An HTML interface has been developed for database access, which will later be integrated into the hardware–software system, thereby ensuring convenient remote user access to the data. As an alternative interface for working with the database, the Anytype software has been employed. Anytype is a NoSQL database management system that utilizes graph-based and document-oriented data models for storing and synchronizing information in a distributed environment. The database has a hierarchical structure, which enables efficient navigation to the required experiment and related information (Fig. 1).

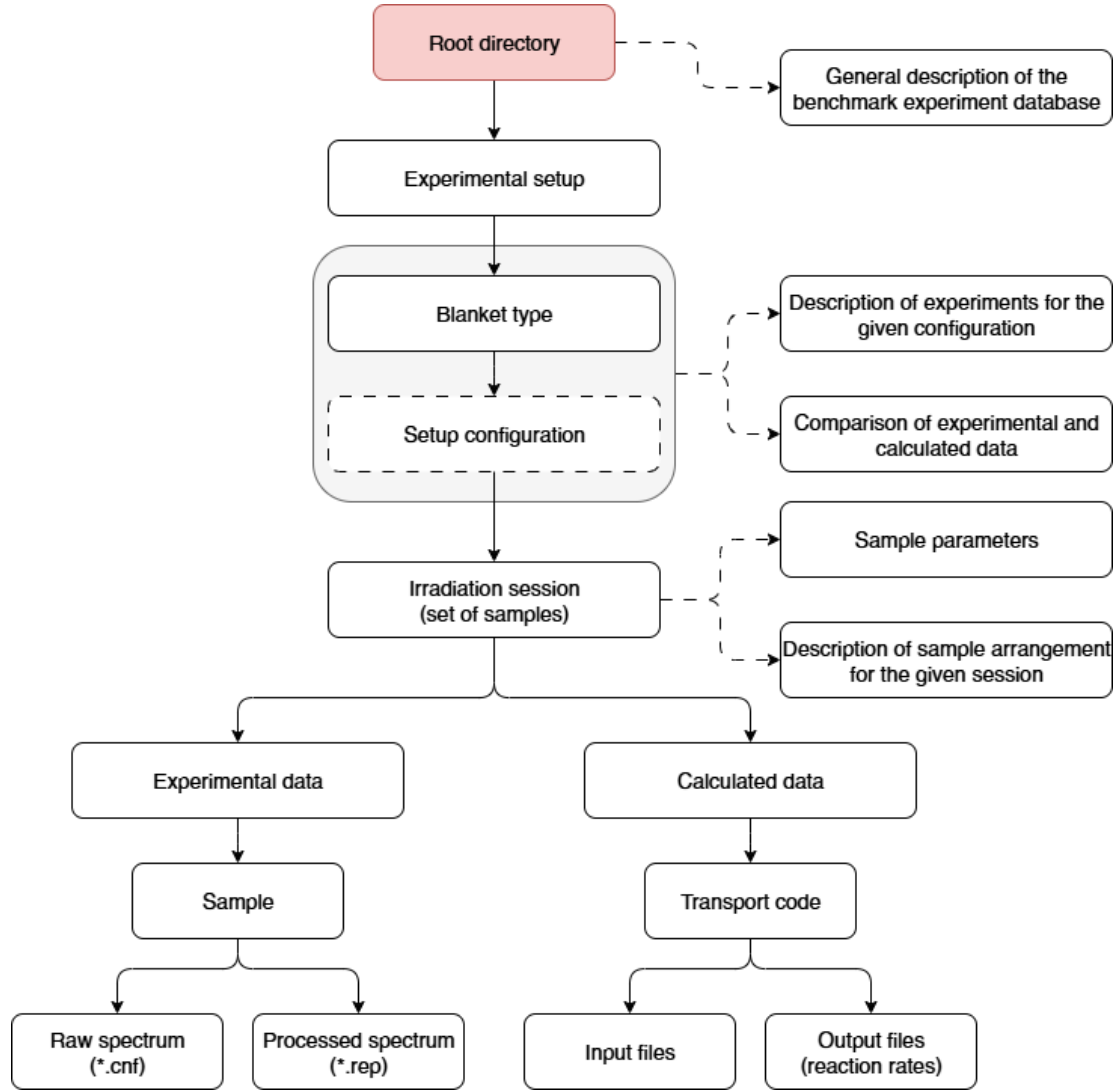


FIG. 1. Structure of benchmark experiments database

2.2. Evaluated nuclear data database

Within the second direction of the unified database development, a hardware–software system – the Visualizer of Fusion-Controlled Data System (VISTUD) – is being designed. The system is designed for the storage, transformation, analysis, and visualization of existing neutron fusion data, with a focus on the use of modern data libraries (ENDF [9], ROSFOND [10], etc.) and processing codes (GRUCON [11], NJOY [12], and others), as well as analysis and visualization tools.

The developed hardware–software system addresses the following tasks:

- storage of fusion-related data, including in compressed formats;
- storage of metadata on nuclear data, results of analysis and visualization, as well as associated service information;
- transformation of nuclear data;
- analysis (including comparative) and visualization of nuclear data;
- export of required nuclear data into various formats (e.g., ACE [13]);
- user interaction via a web interface in local networks and the Internet.

The conceptual scheme of interaction with the VISTUD hardware–software system is presented in Fig. 2.

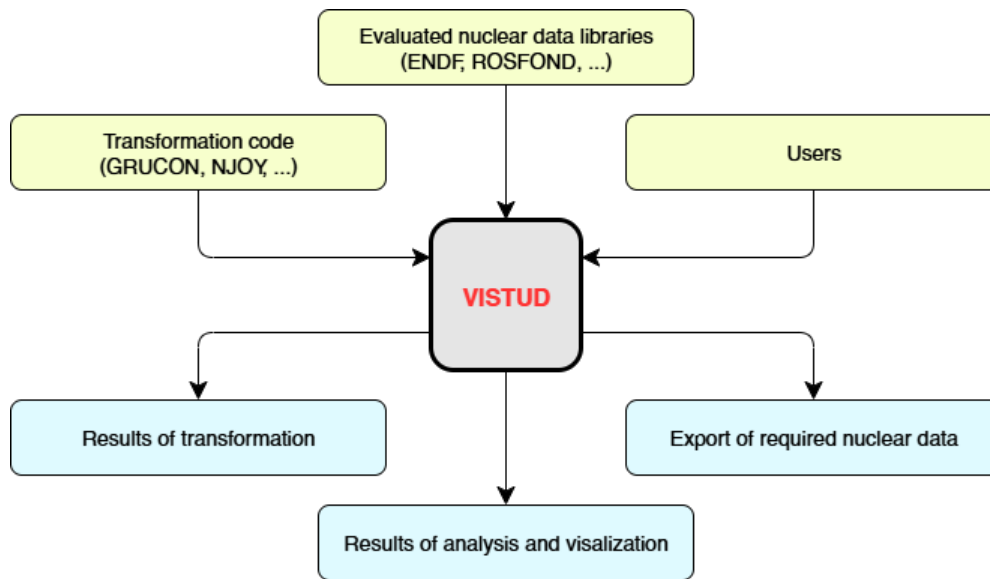


FIG. 2. The conceptual scheme of interaction with the VISTUD hardware–software system

The developed system must meet the following requirements, the implementation of which is mostly determined by the hardware and by the capabilities of the hosting platform:

- data scalability, ensuring the possibility of building a comprehensive nuclear data library;
- computational scalability, allowing the increase in the number of tasks processed simultaneously and enabling interactive operation;
- regular data backup, which may be implemented using the infrastructure of the hosting facility.

The VISTUD hardware–software system consists of subsystems for management, data storage, computation, user interaction, and auxiliary infrastructure:

- the management subsystem includes the control module and the system registry database;
- the data storage subsystem comprises the database and a file server;
- the computational subsystem integrates modules for control, data transformation, export, visualization, and analysis of results;
- the user interface subsystem provides both a local interface and a web interface for operating the VISTUD system within local networks and over the Internet, with support for authorized access;
- the auxiliary infrastructure includes additional computational resources and a backup system.

The structure of the VISTUD hardware–software system is shown in Fig. 3.

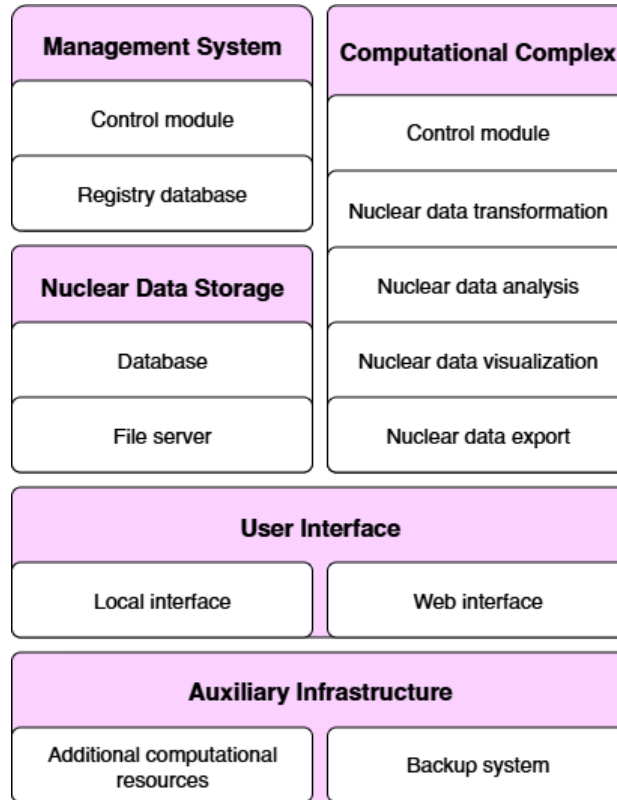


FIG. 3. The structure of the VISTUD hardware–software system

The general architecture, design, and prototype of the VISTUD hardware–software system have been developed. The prototype includes a single-threaded control module (with a command interface and a registry database), as well as subsystems for data storage (with a database and tools for data population and access) and for data transformation (with preliminary adaptation and verification of the GRUCON code for operation within the system). The database has been partially populated using the ROSFOND library. Interfaces for interaction with the control module have been implemented for all subsystems developed.

The VISTUD hardware–software system is being built on a modern technological stack, including modern versions of SQL (PostgreSQL), Python, and C++. The software is intended to operate under 64-bit Linux operating systems (with kernel version 5.3 or higher, supporting the MPI standard).

At present, a multithreaded control module and a web interface for full-scale operation of VISTUD are under development. Subsystems for data analysis, export, and visualization are planned, followed by their integration into the complex. For permanent operation, deployment of a fully functional version populated with data on scalable hardware with authorized access is envisaged.

The ultimate goal of the project is the implementation of a hardware–software system scalable in terms of data volume, computational resources, and functionality, providing efficient work with fusion data.

2.3. Materials database

Within the third direction, data on the properties of materials of interest for the NRC “Kurchatov institute” project on the development of a hybrid reactor have been compiled into a database. The structure of the database and content is quite analogous to the materials database developed for the ITER project [14]. The database primarily contains information on Russian materials, as well as materials developed within the framework of international collaborations involving Russian participation.

At the present stage of work on the database of structural and functional material properties for hybrid systems, the following elements have been developed:

- a hierarchical structure;

- data formats;
- element codification;
- templates for data preparation prior to entry;
- tools for populating and accessing the database;
- a data population methodology based on quality control at each stage of data processing to ensure integrity, formatting, and codification;
- an HTML-based interface providing convenient navigation through sections and subsections when searching for user-required data.

The hierarchical structure of the shell and the navigation scheme are shown in Fig. 4.

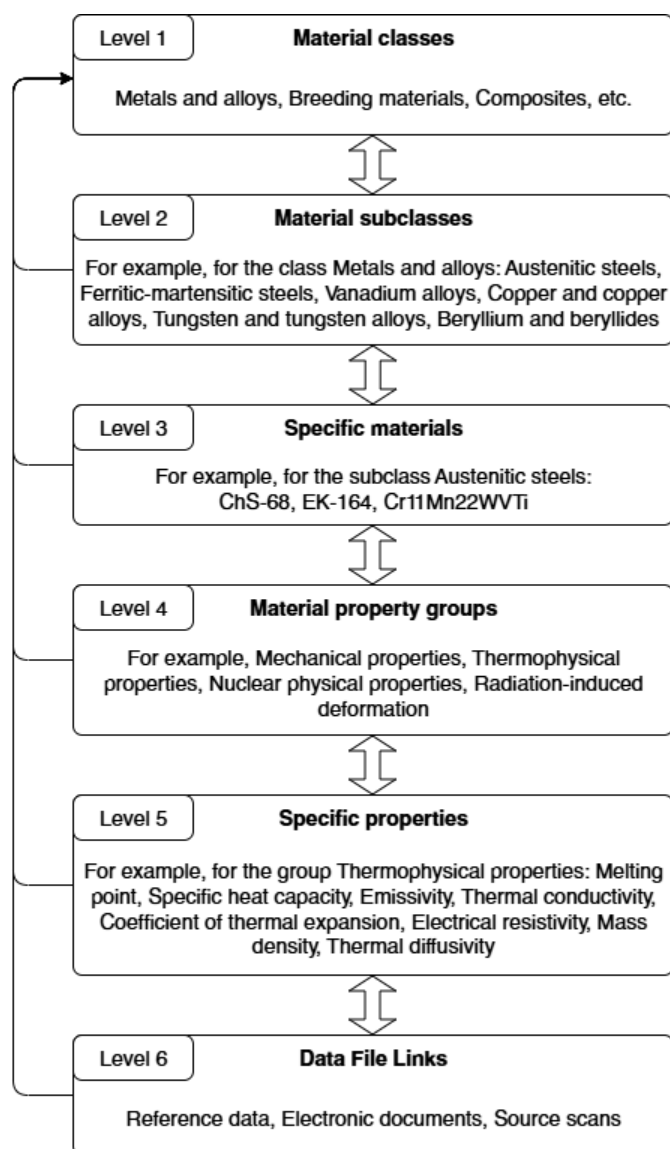


FIG 4. The hierarchical structure of the HTML shell for the database on materials and the navigation scheme.

The database is populated with information from open sources and from research and development results. Graphical data from original publications are digitized manually, while tabular data are processed using artificial intelligence-based tools as well as Python scripts employing specialized libraries.

For user convenience, each dataset associated with a specific property of a given material is accompanied by a reference description, including citations to the original publications. At present, the database contains data on the properties of industrial reactor steels (the chromium–nickel austenitic steel ChS-68, the low-activation

ferritic–martensitic steel Rusfer-EK-181), as well as advanced steels and alloys (the low-activation austenitic chromium–manganese steel of the Cr11Mn22WVTi type, the vanadium alloy V-4Ti-4Cr, and others).

The material properties in the database are grouped into seven categories (Table 1).

TABLE 1. GROUPS OF MATERIAL PROPERTIES

Group code	Group name
1	Introduction
2	Mechanical properties
3	Thermophysical properties
4	Corrosion properties
5	Radiation-induced deformation
6	Interaction with hydrogen and helium
7	Nuclear physical properties
8	Magnetic properties

The “Mechanical Properties” group contains data on short-term and long-term mechanical characteristics, fracture toughness and crack resistance data, as well as the material's elastic properties.

The “Thermophysical Properties” group contains data on the coefficient of thermal expansion, thermal conductivity, thermal diffusivity, specific heat capacity, mass density, melting point, electrical resistivity, and emissivity coefficient.

The “Corrosion Properties” group contains data on corrosion resistance and material behavior in environments of interest.

The “Radiation-Induced Dimensional Change” group contains information on radiation creep and radiation swelling of materials under damaging neutron irradiation.

The “Interaction with Hydrogen and Helium” group contains information on the sputtering of plasma-facing materials under plasma impact, hydrogen retention and permeation through materials, and the influence of hydrogen and helium on material properties.

The “Nuclear-Physical Properties” group contains data on the material's compositional inventory prior to irradiation, considered neutron spectra, information on the calculation code and nuclear data libraries used, and calculated data for materials irradiated for extended periods in fission and fusion nuclear reactors, including long post-irradiation cooling times (accounting for radioactive elements of many generations):

- activation and transmutation of elements defining the material's composition (matrix, alloying, impurity);
- production (concentrations) of gaseous elements: H, ^3H , He, ^{14}C , O, N;
- gamma-ray equivalent dose rate (Sv/h);
- radioactivity (Bq/kg);
- nuclear heat production during and after irradiation (W/kg);
- neutron absorption in all possible types of nuclear reactions;
- isotopes defining the gamma dose rate, radioactivity, and heat production.

The “Magnetic Properties” group contains data on magnetic susceptibility and other magnetic properties of materials.

3. CONCLUSION

A benchmark experiment database has been developed for the verification of evaluated nuclear data libraries and transport codes, as well as a database on the properties of structural and functional materials. The VISTUD hardware–software system is currently at the stage of user interface development and refinement of the remaining subsystems. These databases are intended to support the design of a fusion neutron source. Their integration into a unified management system is envisaged. All databases are continuously being populated with target data, and tools for their processing are under development. The resulting system is expected to enhance the efficiency and safety of developing technical solutions in the design of a hybrid reactor.

ACKNOWLEDGEMENTS

The calculations were carried out using the equipment of the Center for Collective Use “Complex for Modeling and Data Processing of MegaClass Research Facilities” of the National Research Center “Kurchatov Institute”

REFERENCES

- [1] STACEY, W.M., Transmutation missions for fusion neutron sources, *Fusion Engineering and Design* 82 1 (2007) 11.
- [2] KUTEEV, B.V., GONCHAROV, P.R., Fusion–Fission Hybrid Systems: Yesterday, Today, and Tomorrow, *Fusion Science and Technology* 76 7 (2020) 836.
- [3] TITARENKO, Yu.E. et al., Verification of nuclear data libraries used to design molten salt blankets of a fusion neutron source, *Annals of Nuclear Energy* 211 (2025) 110983.
- [4] KHRIPUNOV, V., First wall material damage induced by fusion-fission neutron environment, *Fusion Engineering and Design* 109–111 (2016) 7.
- [5] BLOKHIN, A.I., CHERNOV, V.M., Nuclear physical properties of austenitic nickel and manganese steels under neutron irradiation in nuclear fission (fast) and fusion reactors, *Problems of Atomic Science and Technology, Ser. Thermonuclear Fusion* 43 3 (2020) 11.
- [6] TITARENKO, Yu.E. et al., Benchmark Experiments for Verification of Nuclear Data Libraries for Designing Fusion Blankets, *Fusion Science and Technology* 78 7 (2022) 549.
- [7] TITARENKO, Yu.E. et al., Benchmark Experiments Methodology on Base the Neutron Generator NG-24M and Micromodels of the Fusion Neutron Source (FNS), *Problems of Atomic Science and Technology, Ser. Nuclear And Reactor Constants* 2 (2023) 60.
- [8] TITARENKO, Y.E. et al., Radiation and Nuclear Physics Aspects of the Use of the Thorium Fuel Cycle in a Hybrid Fusion Facility, *Fusion Science and Technology* 79 2 (2023) 117.
- [9] Evaluated Nuclear Data File (ENDF),
<https://www-nds.iaea.org/exfor/endl.htm>
- [10] NIKOLAEV, M.N., ROSFOND – Russian national library of evaluated neutron data,
<https://www.ippe.ru/reactors/reactor-constants-datacenter/rosfond-neutron-database>
- [11] SINITSIN, V.V., The GRUCON code package for Evaluated Nuclear Data Processing. User manual (2021),
<https://www-nds.iaea.org/grucon/>
- [12] MACFARLANE, R.E., MUIR, D.W., BOICOURT, R.M., KAHLER, A.C., The NJOY Nuclear Data Processing System, Version 2012. Theoretical Division Los Alamos National Laboratory. LA-UR-12-27079. (2012).
- [13] A Compact ENDF (ACE),
<https://github.com/NuclearData/ACEFormat>
- [14] DAVIS, J.W., SMITH, P.D., ITER material properties handbook, *J. Nucl. Mater.* 233–237 2 (1996) 1593–1596.