DESCRIPTION OF WIMS LIBRARY UPDATE PROJECT (WLUP)

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Abstract

WIMS-D is one of the few reactor lattice codes that are in the public domain and therefore are available on non-commercial terms, for research and power nuclear reactor calculations. The main weakness of the WIMS-D package is its multi-group constants library, which is based on very old data. Relatively good performance of WIMS-D is attributed to a series of empirical adjustments to the multi-group data. However, the adjustments are not always justified by more accurate and recent experimental measurements. In view of the recently available new, or revised, evaluated nuclear data files it was felt that the performance of WIMS-D could be improved by updating its library. The WIMS-D Library Update Project (WLUP) was initiated in the early 1990´s and finished in 2001. The International Atomic Energy Agency (IAEA) supported its co-ordination, but the project itself consisted of voluntary contributions from a large number of participants. In due course, several benchmarks for testing the library were identified and analyzed, the WIMSR module of the NJOY code system was upgraded, a detailed parametric study was performed to investigate the effects of various data processing input options on integral results and, the data processing methods for the main reactor materials were optimized. The final product, available on CD-ROM from NDS-IAEA includes: 69 and 172 group WIMSD libraries prepared from the selected evaluated data files, IAEA-TECDOC with detailed documentation, Processing inputs, Benchmark inputs and, the system of auxiliary codes developed under the project.

I. INTRODUCTION AND SUMMARY OF THE PROJECT

The WIMS-D code [1] is a freely available thermal reactor physics lattice-cell code used widely especially by scientists in developing countries for thermal research and power reactor calculations.
In 1998, the WIMSD-5B version of the code has been released from the OECD/NEA Data Bank [2}. An important improvement of this version lies on the inclusion of the “1986” WIMS-library [3]. The UK has significantly improved the WIMS nuclear data library since 1986 but the improved versions are not freely available.
The WLUP assumes special importance because of the need to provide updated working libraries compatible with the WIMS codes or equivalent lattice cell codes that are compatible with WIMS-D nuclear data working library.
The preparation of updated working WIMS-D libraries is an important practical step that enables scientists and reactor designers to make use of the most recent evaluated nuclear data files for research and power thermal reactor calculations.
WLUP started officially in the early 90's [4]. In 1996 set up WLUP as a Co-ordinated Research Project (CRP). The final stage of WLUP begin in December 1998, with research contracts issued to participants. Research Co-ordination Meetings were held in Vienna, Austria (1999), Bariloche, Argentina (2000) and Vienna, Austria (2001), with the participation of scientists from 11 laboratories of different IAEA Member States. During the last few years intensive work was performed. All the objectives were achieved. The present document refers to the final results of WLUP.

SUMMARY OF WORK

Work before the CRP

From the beginning, the project was divided into several stages. On stage 1, extensive work was performed to define benchmarks. This was a crucial step in the project in which more than 20 laboratories participated. Five light water moderated Uranium metal and Uranium oxide lattices were specified. Stage 2 was to check the definitions of the multi-group constants in the WIMS library and to upgrade the data processing codes. On stage 3, the main reactor materials in the existing WIMS-D library were replaced for testing purposes. After an extensive parametric study to investigate the effects of various data processing options on the integral benchmark results, NJOY inputs for the main reactor materials were optimized. Stage 4-6 were to replace the actinides and fission-products cross sections, fission product yields, decay and burnup data, the structural materials, and other moderators and add missing materials for different applications. Stage 7 was to complete benchmark testing and prepare the library documentation.

Several procedures and auxiliary programs were implemented during the different steps of the project to simplify the data processing task and input file maintenance

Work during the CRP

The main objective was to produce the following material:

1. A fully updated WIMS-D library, compatible with the WIMSD5B code.
2. A users guide, providing necessary documentation for the updated library.

To allow the updating procedure to be repeated based on any other evaluated data library, the following products were also required:

3. NJOY input instructions for one or more of the major evaluated nuclear data libraries.
4. Automatic procedures for updating the WIMS-D library under one or more computer platforms.
5. Documentation describing the data processing methods and assumptions.

The secondary objective was to remove the restriction in the WIMS-D code which limits the data to 69 energy groups. The library could then be reassembled with a larger number of groups.

Due to different interests the final product of the project was not only a single recommended WIMS-D library, but also a set of recommended inputs for data processing, library updating, verification and validation. The inputs are applicable to a variety of currently available (and future releases) of the basic evaluated nuclear data files and to different applications of the WIMS code. As a by-product of course, the libraries based on various data files were produced also and made available to the users.

Maintenance and promotion of the final product

The official generic name of the library is WIMSD-IAEA.

The library exists in two group structures: WIMSD-IAEA-69 in 69 energy groups and WIMSD-IAEA-172 in 172 energy groups.

The Agency will package and distribute the CRP final product, which includes libraries and documentation to users in Member States.

The Agency should collect feedback from the users and provide for future updates to fulfil the requirements of the users or when new evaluated data become available.

The WIMSD-IAEA and other libraries generated on WLUP and all the material related with the generation of libraries and benchmarks will be available from the Web server of. IAEA-Nuclear Data Section. A CD-ROM with all this material and additional valuable information will be also available upon request.

II. MAIN FEATURES

PARAMETERS INCLUDED IN THE LIBRARY

The main parameters included into the WIMSD library are the transport, absorption and fission cross sections (for fissile isotopes), the P1 transport corrected P0 scattering matrix and resonance integrals (for resonance isotopes).
Other parameters are: potential cross section, slowing-down power per unit lethargy, fission neutron production cross section, fission product, burnup and actinide chain data, fission spectrum and P1-matrix for the main moderators.
Smooth cross sections in the thermal energy range and resonance integrals in the resonant energy range are temperature dependent. Multi-group cross sections are produced from pointwise cross sections included in evaluated nuclear data files by weighting with appropriated energy spectra.
The Main improvements on cross sections and related parameters are:
-Self-shielding of scattering cross sections with typical dilutions
-Goldstein-Cohen factors re-calculated with detailed method
-Three different condensation neutron spectra (for LWR, HWR and ThO2-D2O systems)
-Two different neutron current for transport correction (for H2O and D2O moderators)
-Extended number of temperatures for thermal data.

RESONANCE TREATMENT AND GOLDSTEIN-COHEN LAMBDA FACTORS

The resonance treatment method based on equivalence theorems, included in WIMSD program, requires resonance integrals in function of background cross sections, and the Goldstein-Cohen 'lambda-factors' for each material.
In the frame of WLUP, the NRSC system of codes was developed to estimate the Goldstein-Cohen parameter λ following the WIMSD conventions for the main materials [5]. The objective of this work was the development of the capacity for calculating the lambda factors from any set of basic nuclear data file, following the WIMSD formalism of resonance treatment.
The system NRSC is included on the WLUP CD-ROM.
The Main improvements on resonance integrals are:
-Extended number of temperatures for Doppler effect
-Background cross sections revised for better interpolation between tabulated values.

SELECTION OF EXPLICITLY REPRESENTED AND LUMPED FISSION PRODUCTS

The nuclear fission process in the fuel of a nuclear reactor core causes accumulation of fission products. Some of them influence the nuclear properties of the core very strongly and must be treated explicitly. Others - although individually unimportant - have a cumulative effect, which can-not be neglected. Usually they are lumped into a pseudo fission product.
In the frame of the WIMS-D Library Update Project (WLUP) a set of criteria was developed to select the fission product candidates. Following these criteria 56 nuclides were explicitly represented in the library and 79 nuclides were lumped into a pseudo fission product.
Based on the analytical equations that govern the build-up and decay of the fission products a set of quantitative criteria was developed [6].

MATERIALS

173 materials are included in the WIMSD-IAEA libraries. Each material is identified with an integer ID number, usually consisting of 1-4 digits. The numbers are the same as in the WIMS86 library for all materials included in that library.
Thermal data are given at several temperatures.
Materials are classified by type: moderators, structural materials and other components, dosimetry reactions (to be used for calculating reaction rates only), fission products, fissile and fertile actinides and burnable materials.
Regarding the source of evaluated data for each material included in the 69 and 172 group WIMSD-IAEA libraries, the selection was performed taking into account the evaluations included in the FOND-2 library and JEFF-3T starter file, as well as, the results of analysis of more than 200 benchmark cases for different libraries in the frame of WLUP. The references to the different evaluated data files processed within WLUP are [7-11].

Table 1. Number of materials by type included in the libraries

Library	WIMS86[3]	IAEA
Total number of materials	129	173
Moderators	3	5
Fission products	36	58
Burnable absorbers	18	20
Resonant materials	14	28
Actinides	18	21
Dosimetry reactions	11	37

DOSIMETRY DATA

The dosimetry data are included in the WIMS-D library as special materials to perform reaction rate calculations using the WIMS-D lattice code. A total of 15 dosimetry materials are contained in the '1986' WIMS library. They include 8 dosimetry reactions, 2 damage cross-sections and 5 additional materials that are useful for special cases as a "1/v" absorber, a constant absorber and the inverse lethargy intervals.
In the frame of WIMS Library Update Project all the dosimetry files were updated from recently evaluated nuclear data files. Additionally, 22 new dosimetry reactions were included in the library for the 69 and the 172 energy structures. They are 14 different dosimetry reactions and the (n,2n) reaction for major actinides.

BURNUP DATA

In Fig.I, a graphical description of the actinides burnup and decay transitions implemented in WIMSD-IAEA libraries is given. In Fig.II, the fission product chains are shown,
The Main improvements on burnup chains are [12,13]:
-Special treatments for U232,U237 production simulation
-Special treatment of capture and decay of Am isotopes.
-Update the fission product yields and decay data
-22 new fission products explicitly included

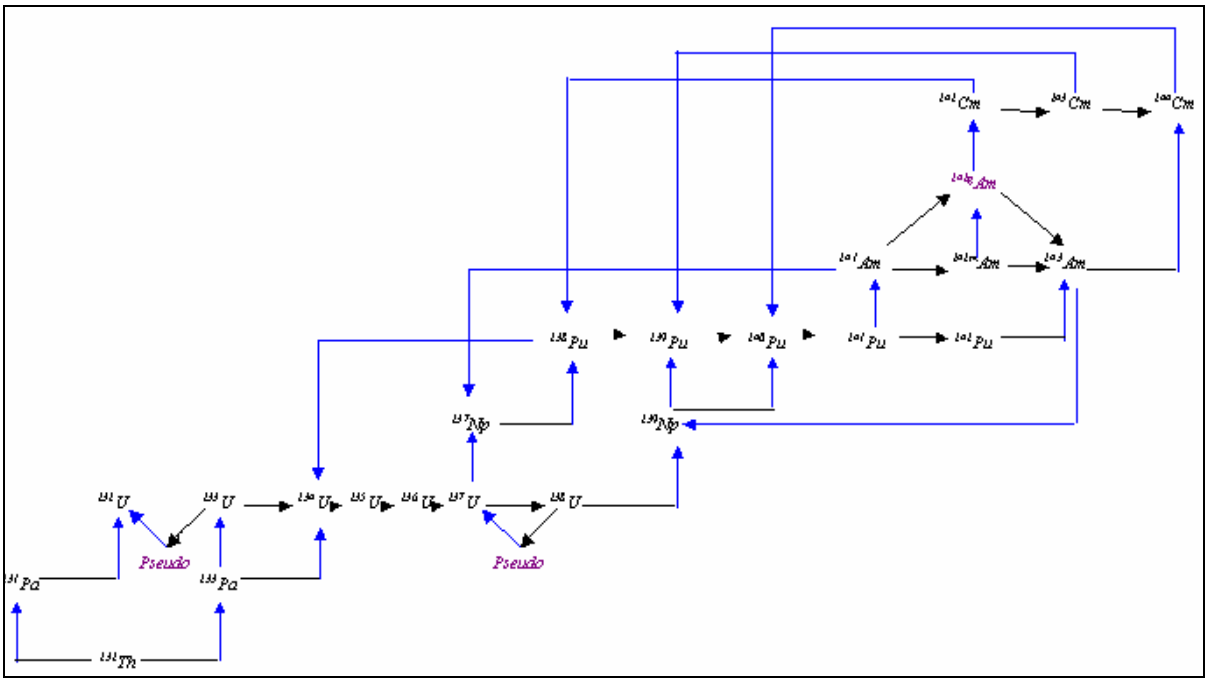

Figure I. Actinide chain

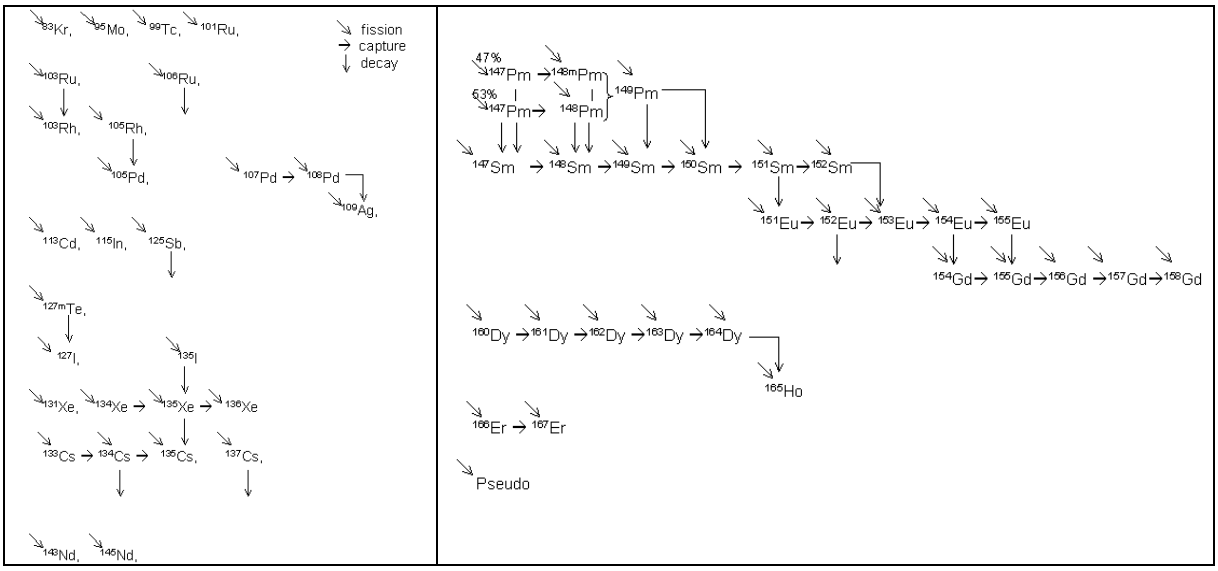

Figure II. Fission Product Chains

AVERAGING FLUX AND CURRENT SPECTRA

The adopted neutron spectrum in WLUP was essentially the standard PWR spectrum included in the GROUPR module of NJOY [14], with a modification to smooth the form to a pure 1/E function on the resonance energy region, where special resonance treatment is made for main resonance materials.
For HWR's, a special spectrum has been generated with MCNP code [15], used for deuterium data only.
For systems using thorium fuel cycle, another special spectrum has been generated with MCNP code, used for thorium-232, protoactinium-231 and uranium-233 data only.
Besides, on the formalism of multi-group libraries, a neutron current spectrum is necessary for obtaining the 'transport correction' from P1 cross section data. The correction is made by weighting P1 cross-sections with a 'typical' neutron current spectrum. The selection of the weight spectrum for this process is simplified by choosing the "British current spectrum", a reference spectrum from the old WIMS library generations. This current is adopted for generation of WLUP-69 group libraries, with the exception of deuterium data. For this isotope, and for 172 group libraries, the necessary multi-group neutron current spectrum has been generated by solving the B1 equations for typical LWR and HWR cases [16].

ENERGY STRUCTURE

69 group library
The original WIMSD structure is used, with 14 fast groups between 10 MeV and 9.118 KeV, 13 resonance groups between 9.118 KeV and 4 eV, and 42 thermal groups from 4 and 0 eV.

172 group library
The structure of new commercial WIMS libraries is adopted, with 45 fast groups between 19.64 MeV and 9.119 KeV, 47 resonance groups between 9.119 KeV and 4 eV and 80 thermal groups from 4 and 10^{-5} eV.

Table 2. Number of energy groups by type included in the libraries

Library	WIMS86,IAEA69	IAEA172
Fast groups	14	45
Resonance groups	13	47
Thermal groups	42	80
Total	69	172

WIMSD-5B EXTENSIONS

The major modifications and extensions are [17]:
1) Upper limit of 200 energy groups (before: 69 groups)
2) Extended upper energy of the first fast group: 20 MeV (before: 10 MeV)
3) Up to 55 resonance groups (before: 13 resonance groups)
4) Up to 30 resonant isotopes
5) Up to 300 burnable nuclides from the library
6) Up to 60 burnable materials in WIMSD input
7) Modification to treat WIMS-D libraries with extended format that includes multiple product-nuclei reactions.

EVALUATED NUCLEAR DATA PROCESSING OPTIONS

The main codes used for data processing are:
- NJOY Nuclear Data Processing System (Version 99.65) to generate multigroup constants for WIMSD from the evaluated nuclear data files [14].
- AVRFPY code to process fission product yield and decay data.
- WILLIE code to manage the WIMSD library.
- NRSC system of codes to calculate the Goldstein-Cohen parameters.
- ENDF Pre-Processing codes to process dosimetry cross sections.
- WIMSIE to convert PrePro output for dosimetry reactions into WIMSD format.
- XnWlup for interactive visualisation of the cross sections in the WIMSD libraries.

In addition, there exists a number of utility codes for performing minor data manipulation, post-processing of WIMSD code outputs, sorting and comparing the results.

III. BENCHMARKS

A set of well documented benchmarks has been selected with the following objectives:
a) tests of the performance of new WIMSD libraries generated by WLUP,
b) comparison of results obtained with libraries generated from different basic nuclear data,
c) detection of tendencies in the discrepancies in the results for the main materials.
There are two sequences of benchmarks: standard and supplementary benchmarks. The standard sequence of tests includes a set of benchmarks that can be analyzed using just the WIMSD code. The supplementary sequence of benchmarks includes cases that may require additional processing like cross section homogenization, whole core calculations, etc. and other benchmarks incorporated at the last minute.
The standard sequence of benchmarks are classified in two categories:
1) criticality experimental benchmarks (main parameter compared: Keff),
2) burnup benchmarks (main parameters compared: isotopic concentrations of actinides and fission products as a function of burnup).
WIMS inputs, reference solution, post-processing codes and batch files for running WLUP benchmarks and graphs of leakage spectrum for each benchmark are included in WLUP CD-ROM.

Standard benchmark groups	**#benchmarks**	**#cases**
1) H2O-moderated uranium metal lattices	6	64
2) H2O-moderated uranium oxide critical lattices	14	57
3) WWER-type UO2-H2O critical lattices	1	25
4) H2O-moderated UO2-PuO2 (MOX) critical lattices	4	40
5) Uranium intermediate spectrum critical homogeneous system	1	1
5) Plutonium intermediate spectrum critical homogeneous system	1	1
6) H2O-moderated $^{233}UO2$-ThO_2 lattices	1	8
7) D2O-moderated $^{233}UO2$-ThO_2 lattices	1	8
8) D2O-moderated uranium oxide critical lattices	4	11
9) D2O-moderated ^{235}UO2-ThO2 critical lattices	1	4
total:	24	219

Standard burnup benchmarks

Analysis of isotopic composition as a function of burnup :

1) NPD. 19-rod Fuel Clusters. D2O-moderated uranium oxide lattices.
2) NEA Burnup Credit Criticality Benchmark H2O-moderated uranium oxide lattices.
3) LWR-Pu Recycling Benchmarks. H2O-moderated mixed oxide lattices.

Main sources of experimental results and references

A large amount of information included on UME-LW, UO2-LW and MOX-LW benchmarks has been retrieved from the compilation edited by E.Bernocchi and R.Martinelli [18] and from original publications of the experimentalists referenced in this publication. Other references are [19-23].

In the following table, a resume of standard criticality benchmark results for WIMSD-IAEA 172 library is given. The WIMS86 library results are included also, to see the differences of the new non-adjusted libraries compared to the old adjusted one.

Table 2. Average results of standard criticality benchmarks (*)

Uranium criticality benchmarks (64 cases)

Case	DK-eff	SD	DRho28	SD	DDel25	SD	DDel28	SD	DConvR	SD
Exp.	0.24		1.76		1.17		4.71		0.97	
Iaea172	-0.02	0.72	3.05	0.31	-1.29	0.60	3.61	1.19	0.21	0.21
Wims86	-0.09	0.62	2.11	0.56	-1.36	0.54	5.33	1.35	0.66	0.24

Uranium UO2 criticality benchmarks (57 cases)

Case	DK-eff	SD	DRho28	SD	DDel25	SD	DDel28	SD	DConvR	SD
Exp.	0.29		3.05		9.24		7.00		2.75	
Iaea172	-0.30	0.68	3.28	2.50	-0.76	1.05	0.41	6.40	1.89	1.78
Wims86	-0.74	0.69	3.00	2.35	-1.07	1.17	2.53	6.32	1.93	1.94

WWER criticality benchmarks (25 cases)

Case	DK-eff	SD
Exp.	0.56	
Iaea172	-0.33	0.75
Wims86	-0.84	0.97

LWR MOX criticality benchmarks (40 cases)

Case	DK-eff	SD
Exp.	0.19	
Iaea172	0.00	0.72
Wims86	-0.05	0.68

Uranium intermediate spectrum critical homogeneous systems (1 case)

Case	DK-eff
Exp.	0.10
Iaea172	3.06
Wims86	-0.59

Plutonium intermediate spectrum critical homogeneous systems (1 case)

Case	DK-eff
Exp.	0.10
Iaea172	1.59
Wims86	4.17

BNL-Th2-U3-H2O criticality benchmarks (8 cases)

Case	DK-eff	SD	DRho28	SD
Exp.	0.45		3.66	
Iaea172	0.69	0.35	-16.60	2.15
Wims86	-0.54	0.14	-9.83	2.13

BNL-Th2-U3-D2O criticality benchmarks (8 cases)

Case	DK-eff	SD	DRho28	SD	DDel28	SD
Exp.	0.58		5.35		11.90	
Iaea172	-0.18	1.16	-7.41	6.90	-4.51	4.41
Wims-86	-2.21	0.77	0.43	6.83	-9.63	4.87

Uranium D2O criticality benchmarks (15 cases)

Case	DK-eff	SD	DRho28	SD	DDel25	SD	DDel28	SD	DConvR	SD
Exp.	0.24		5.8		0.5		1.00		0.40	
Iaea172	0.26	0.43	16.2	25.7	-2.0	2.9	0.73	0.74	1.17	1.17
Wims-86	0.02	0.28	11.9	19.2	-1.5	2.3	0.87	0.98	0.05	0.29

(*) Keff: Effective multiplication factor;

Rho28: ρ^{28} : ratio of epithermal to thermal U-238 capture reaction rate

Del25: δ^{25} : ratio of epithermal to thermal U-235 fission reaction rate

Del28: δ^{28} : ratio of U-238 fission to U-235 fission reaction rate

ConvR: C^{*} : ratio of U-238 capture to U-235 fission reaction rate

DK-eff, DRho28, DDel25, DDel28,DConvR: calc/exp. in % (average value over all cases)

SD: Standard deviation ratio, in %, of each parameter to the left.

VI. CONCLUSIONS AND RECOMENDATIONS

The original and main objective of WLUP, the production of an updated and tested WIMSD multigroup data library, has been accomplished.
The results from benchmark tests show good performance of the final library with respect to experimental results of different parameters and other adjusted libraries such as WIMS86, i.e.-the library that is included with the WIMSD-5B package. The WIMSD-IAEA libraries are not adjusted from integral experiments. The nuclear data processing was performed based on general reactor physics principles and following the WIMS-D model conventions.
The benchmark tests prepared for WLUP and used for testing the partials and the final library, include more that 200 cases for more than 10 different systems and combinations of fuels, moderators and geometry, for different conditions and parameters.
The original objective was enhanced with the generation of a library at 172 energy groups, besides the standard 69 groups. The modifications to WIMSD-5B original code to make possible the use of the 172 group library were also successfully prepared.
A set of programs and batch files were developed for generation of the libraries and for running the benchmarks cases. All this material is included on a CD-ROM and WEB-page for free use.
The users of multigroup libraries now have the possibility of generating their own libraries with the methods and procedures given in WLUP.
A better understanding of the physics and methods included in multigroup data libraries, in transport codes such as WIMSD and in the basic nuclear data files and the processing methods.
The new libraries present improvements on several parameters with respect to the last freely available WIMSD library before WLUP (WIMS86).

SUGGESTIONS FOR FUTURE IAEA ACTIVITY ON THE SUBJECT

- In two-year time (2003 or 2004) to organize a Consultant Meeting regarding feedback on the WIMSD-IAEA library.
- Maintain a WEB page for WIMSD-IAEA Library including information on feedback from users.
- Evaluate the possibility for organising a CRP on research reactors calculations. It could be a good opportunity to promote the WIMSD-IAEA library for global calculations.
- Include scripts and programs to run under UNIX.
- Implement extended burnup schemes into the libraries.
- Include JENDL3.3 and CENDL3 based libraries.
- Revise IAEA libraries as necessary.
- Add new benchmarks (include more full core cases).
- Perform deep analysis of benchmark results.
- Implement further improvements to WIMSD code.

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