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**Benchmark for Uncertainty Analysis in Modelling (UAM)
for Design, Operation and Safety Analysis of LWRs**

Volume I: Specification and Support Data for the Neutronics Cases (Phase I)

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NUCLEAR ENERGY AGENCY
NUCLEAR SCIENCE COMMITTEE
NEA COMMITTEE ON SAFETY OF NUCLEAR INSTALLATIONS

**BENCHMARK FOR UNCERTAINTY
ANALYSIS IN MODELING (UAM) FOR DESIGN,
OPERATION AND SAFETY ANALYSIS OF LWRs**

*Volume I: Specification and Support Data
for the Neutronics Cases (Phase I)*

Version 1.0

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Foreword

In recent years there has been an increasing demand from nuclear research, industry, safety and regulation for best estimate predictions to be provided with their confidence bounds. Consequently an "in-depth" discussion on "Uncertainty Analysis in Modeling" was organized at the 2005 OECD/NEA Nuclear Science Committee (NSC) meeting, which led to a proposal for launching an Expert Group on "Uncertainty Analysis in Modeling" and endorsing the organization of a workshop with the aim of defining: future actions and a program of work.

As a result the OECD/NEA Uncertainty Analysis in Modeling (UAM) Workshop took place in Pisa, Italy on April 28-29, 2006. The major outcome of the workshop was to prepare a benchmark work program with steps (exercises) that would be needed to define the uncertainty and modeling tasks. The other proposals made during the meeting were to be incorporated under the different steps (exercises) within the overall benchmark framework for the development of uncertainty analysis methodologies for multi-physics (coupled) and multi-scale simulations.

Following the results of the UAM-2006 Workshop, the OECD/NEA NSC at its June 2006 meeting endorsed the creation of an Expert Group on Uncertainty Analysis methods in Modeling under the auspices of the Working Party on Scientific issues in Reactor Systems (WPRS). Since the Expert Group addresses multi-scale / multi-physics aspects of uncertainty analysis, it works in close co-ordination with the benchmark groups on coupled neutronics/thermal-hydraulics simulations and on coupled core-plant problems. It also coordinates its activities with the Group on Analysis and Management of Accidents (GAMA) of the Committee on Safety of Nuclear Installations (CSNI). The Expert Group has the following mandate:

1. To elaborate a state-of-the-art report on current status and needs of sensitivity and uncertainty analysis (SA/UA) in modeling, with emphasis on multi-physics (coupled) and multi-scale simulations.
2. To identify the opportunities for international co-operation in the uncertainty analysis area that would benefit from coordination by the NEA/NSC.
3. To create a roadmap along with a schedule and organization for the development and validation of methods and codes required for uncertainty analysis including the benchmarks adequate to meet those goals.

The NEA/NSC has endorsed this activity to be undertaken with the Pennsylvania State University (PSU) as the main coordinator and host with the assistance of the Scientific Board. To summarize, in addition to LWR best-estimate calculations for design and safety analysis, the modeling aspects of Uncertainty Analysis (UA) and Sensitivity Analysis (SA) are to be further developed and validated on scientific grounds in support of their performance. There is a need for efficient and powerful UA and SA methods suitable for such complex coupled multi-physics and multi-scale simulations. The proposed benchmark sequence will address this need by integrating the expertise in reactor physics, thermal-hydraulics and reactor system modeling as well as uncertainty and sensitivity analysis, and will contribute to the development and assessment of advanced/optimized uncertainty methods for use in best-estimate reactor simulations. Such an effort can be undertaken within the framework of a program of international co-operation that would benefit from the coordination of the NEA/NSC and from interfacing with the CSNI activities. More information can be found at: <http://www.nea.fr/html/science/egrs/ltb/UAM/>

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Special appreciation goes to the report reviewers, which are the members the Scientific Board of UAM Expert Group:

Scientific Board and Co-ordination

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Chapter 1

INTRODUCTION

In addition to the establishment of Light Water Reactor (LWR) best-estimate calculations for design and safety analysis, understanding uncertainties is important for introducing appropriate design margins and deciding where additional efforts should be undertaken to reduce uncertainties. The need of uncertainty evaluations for LWR best-estimate calculations was discussed and addressed within the framework of the CRISSUE-S international European Union (EU) project [1] along with the identification of sources of uncertainties in coupled neutronics/thermal-hydraulics simulations. For this reason the modeling aspects of Uncertainty Analysis (UA) and Sensitivity Analysis (SA) are to be further developed and validated on scientific grounds in support of their performance. In consequence of recent meetings the international expert community in reactor physics, thermal-hydraulics, and uncertainty and sensitivity analysis, has decided that a first step in this direction is to define an OECD benchmark for Uncertainty Analysis in Modeling (UAM) for design, operation, and safety analysis of LWRs [2, 3, 4]. The expected impact and benefits of the OECD LWR UAM benchmark activity for LWR safety and licensing are summarized in [5]. This benchmark project is challenging and responds to needs of estimating confidence bounds for results from simulations and analysis in real applications.

Reference LWR systems and scenarios for coupled code analysis are defined to study the uncertainty effects for all stages of the system calculations. Measured data from plant operation are available for the chosen scenarios. The existing OECD/NEA/NSC coupled code transient benchmarks – such as BWR Turbine Trip (TT) [6], PWR Main Steam Line Break (MSLB) [7], VVER-1000 (V1000) Coolant Transients (CT) [8], and BWR Full Bundle Test (BFBT) [9] are used as part of the framework for adding uncertainty analysis methodologies in the best estimate modeling for design and operation of LWRs. Such an approach facilitates the benchmark activities since many organizations have already developed input decks and tested their codes on the above-mentioned coupled code benchmarks. From these OECD LWR transient benchmark problems, the Peach Bottom 2 (PB-2) BWR Turbine Trip (TT) is proposed as the first reference system-scenario, although provisions are made to address the other LWR systems and scenarios such as TMI-1 PWR MSLB, PWR-RIA-ATWS, BWR-CRDA-ATWS (with boron modeling), VVER-1000 CT, etc. The Peach Bottom 2 BWR Turbine Trip Benchmark is well documented not only in the OECD/NEA/NRC BWR TT benchmark specifications [6] but also in a series of EPRI [10, 11] and PECO reports [12], which include design, operation, and measured steady state and transient neutronics and thermal-hydraulics data. The fuel cycle depletion, steady state and transient measured data, available at the integral parameter level and the local distribution level, are very important features of the Peach Bottom 2 BWR Turbine Trip. Integration with the OECD/NEA/NRC BWR BFBT benchmark and the uncertainty analysis exercises performed in its framework will be made. The integration of the PB-2 BWR turbine trip will also be extended to the ongoing NEA/CSNI BEMUSE-3 benchmark through the NEA internal co-operation between the NSC and CSNI Committees.

1.1 Objective

The proposed technical approach is to establish a benchmark for uncertainty analysis in best-estimate modeling and coupled multi-physics and multi-scale LWR analysis, using as bases a series of well defined problems with complete sets of input specifications and reference experimental data. The objective is to determine the uncertainty in LWR system calculations at all stages of coupled reactor physics/thermal

hydraulics calculation. The full chain of uncertainty propagation from basic data, engineering uncertainties, across different scales (multi-scale), and physics phenomena (multi-physics) is tested on a number of benchmark exercises for which experimental data is available and for which the power plant details have been released.

The principal objectives are: a) to subdivide the complex system/scenario into several steps or Exercises, each of which can contribute to the total uncertainty of the final coupled system calculation, b) to identify input, output and assumptions for each step, c) to calculate the resulting uncertainty in each step; d) to propagate the uncertainties in an integral systems simulation for which high quality plant experimental data exist for the total assessment of the overall computer code uncertainty. As part of this effort, the development and assessment of different methods or techniques to account for the uncertainties in the calculations will be investigated and reported to the participants.

In summary, the objective of the proposed work is to define, coordinate, conduct, and report an international benchmark for uncertainty analysis in best-estimate coupled code calculations for design, operation, and safety analysis of LWRs. The title of this benchmark is: “OECD UAM LWR Benchmark”.

The experimental data are used as much as possible (two “interactions” with “known” experimental data are indicated above but others can be added). The benchmark team identifies Input (I), Output (O) or target of the analysis, as well as provides guidance on assumptions for each step and target uncertainty parameters (U). The uncertainty from one step should be propagated to the others (as much as feasible and realistic).

1.2 Definition of benchmark phases and exercises

The above-described approach is based on the introduction of 9 steps (Exercises), which allows for developing a benchmark framework which mixes information from the available integral facility and NPP experimental data with analytical and numerical benchmarking. Such an approach compares and assesses current and new uncertainty methods on representative applications and simultaneously benefits from different methodologies to arrive at recommendations and guidelines. These 9 steps (Exercises) are carried out in 3 phases as follows:

Phase I (Neutronics Phase)

- Exercise I-1: Derivation of the multi-group microscopic cross-section libraries (nuclear data plus covariance data, selection of multi-group structure, etc.)
- Exercise I-2: Derivation of the few-group macroscopic cross-section libraries (energy collapsing, spatial homogenization of cross-sections and covariance data, etc.)
- Exercise I-3: Criticality (steady state) stand-alone neutronics calculations with confidence bounds (k_{eff} calculations, diffusion approximation, etc.)

Phase II (Core Phase)

- Exercise II-1: Fuel thermal properties relevant for transient performance
- Exercise II-2: Neutron kinetics stand-alone performance (kinetics data, space-time dependence treatment, etc.)
- Exercise II-3: Thermal-hydraulic fuel bundle performance

Phase III (System Phase)

- Exercise III-1: Coupled neutronics/thermal-hydraulics core performance (coupled steady state, coupled depletion, and coupled core transient with boundary conditions)
- Exercise III-2: Thermal-hydraulics system performance
- Exercise III-3: Coupled neutronics kinetics thermal-hydraulic core/thermal-hydraulic system performance

1.3 Content of this document

Separate Specifications will be prepared for each Phase in order to allow participation in the full Phase or only in a subset of the Exercises. Boundary conditions and necessary input information are provided by the benchmark team. The intention is to follow the calculation scheme for coupled calculations for LWR design and safety analysis established in the nuclear power generation industry and regulation. This specification document covers Phase I¹, which includes the first 3 Exercises (neutronics) as follows:

Chapter 2 of this document provides the definition of Exercise I-1.

Chapter 3 provides the definition of Exercise I-2.

Chapter 4 provides the definition of Exercise I-3.

Chapter 5 specifies the requested output for the three exercises.

Chapter 6 provides summary and conclusions.

This phase is focused on understanding uncertainties in prediction of key reactor core parameters associated with LWR stand-alone neutronics core simulation. Such uncertainties occur due to input data uncertainties, modeling errors, and numerical approximations. Input data for core neutronics calculations primarily include the lattice averaged few group cross-sections. Three main LWR types are selected, based on previous benchmark experiences and available data:

- PWR (TMI-1)
- BWR (Peach Bottom-2)
- VVER-1000 (Kozloduy-6, Kalinin-3)

As a source of their cross-section data the participants can use the Nuclear Data Libraries (NDL), which are normally used in conjunction with their lattice physics codes. The three major libraries (ENDF, JEFF and JENDL) are possible candidates. For cross-section covariance data the 44-group covariance libraries from SCALE-5.1 are proposed. In addition to the covariance matrices, a utility program for interpolating or collapsing from a given group structure to another one is provided for participants' use. Participants can choose any energy multi-group structure according to the input requirements of their lattice code to be utilized.

¹ Please note that the definition of Exercise I-1, provided in this document, is complete. However, the definitions of Exercises I-2 and I-3 might be updated based on experience obtained in performing Exercise I-1 and discussions during incoming benchmark workshops.

For cross-section generation any type of lattice solver can be used. For core calculations the established two-group energy structure for LWR analyses is proposed as the major part of the benchmark activities. However, provisions are made for utilization of other few-group structures if the participants want to investigate them. The Monte-Carlo method will provide reference solutions for the test problems of each Exercise of Phase I.

Chapter 2

DEFINITION OF EXERCISE I-1: CELL PHYSICS

The Exercise I-1 is entitled “Cell Physics”, and is focused on derivation of the multi-group microscopic cross-section libraries. Its objective is to address the uncertainties due to the basic nuclear data as well as the impact of processing the nuclear and covariance data, selection of multi-group structure, and self-shielding treatment. The intention for Exercise I-1 is to propagate the uncertainties in evaluated Nuclear Data Libraries - NDL - (microscopic point-wise cross sections) into multi-group microscopic cross-sections used as an input by their lattice physics codes. The participants can use any of the major NDLs such as Evaluated Nuclear Data Files (ENDF) [13, 14, 15], Joint European Fission and Fusion files (JEFF) [16, 17], and Japanese Evaluated Nuclear Data Library (JENDL) [18]. The evaluation of nuclear data induced uncertainty is possible by the use of nuclear data covariance information. The development of nuclear data covariance files is in progress in major NDLs. For the purposes of the OECD LWR UAM benchmark the availability of covariance data is important for all relevant nuclides (actinides, fission products, absorbers and burnable poisons, structural materials and etc.), present in the reactor core and reflector regions of LWRs, covering the entire energy range of interest (from 0 to 10 MeV), and for all relevant reaction cross-section types.

2.1 Status of nuclear data covariance information

In the major NDLs standards and formats are in place to permit the communication of estimated uncertainties in the evaluated cross-section data. The evaluation of nuclear data induced uncertainty is possible by the use of nuclear data covariance. By including the uncertainty or covariance information, the analyst can propagate cross-section data uncertainties through sensitivity studies to the final calculated quantities of interest. The covariance data files provide the estimated variance for the individual data as well as any correlation that may exist. Availability of covariance evaluations is very limited in the NDLs; however, nuclear data covariance files for some additional materials are being developed for major NDLs. The uncertainty evaluations are developed utilizing information from experimental cross-section data, integral data (critical assemblies), and nuclear models and theory. The covariance information in the NDLs is given in respect to point-wise cross-section data and/or with respect to resonance parameters. Methods to approximate uncertainty data have also been examined, and there are plans to produce a complete set of “low-fidelity” covariance data, which probably will not be included within the official NDLs. This approximate set of data will be distributed for S/U applications with codes such as SCALE.

The uncertainty information in such evaluated libraries is included in files called “covariance files” (files for nuclear variance and covariance data) within the ENDF-6 formalism. The following covariance files are defined:

- Data covariances obtained from parameter covariances and sensitivities (MF30)
- Data covariances for number of neutrons per fission (MF31)
- Data covariances for resonance parameters (MF32)
- Data covariances for reaction cross-sections (MF33)
- Data covariances for angular distributions (MF34)
- Data covariances for energy distributions (MF35)

Data covariances for radionuclide production yields (MF39)

Data covariances for radionuclide production cross-sections (MF40)

To propagate nuclear data uncertainties in reactor core calculations files MF32, MF31, and MF33 are the only data currently available within ENDF/B and other NDL's. For example, for each isotope and type of reaction, quantities in MF33 are the covariances of the expected cross-section values, providing a measure of the accuracy and correlations of the evaluated cross-sections. Please note that the MF33 uncertainties often refer to the *complete* uncertainties in evaluated cross sections, not just uncertainties in the MF3 data. For example, uncertainties in resonance range of a cross section may be described by file 33 whenever file 32 data is not present. The following information is needed for processing uncertainties into the form of full covariance matrices:

- a) Stored quantities in MF3 (or MF 10) - expected value of a physical quantity

$$\langle x \rangle = \int x f(x) dx \quad (1)$$

where $f(x)$ is the density function averaged over all variables other than x .

- b) Stored quantities in MF33 - relative and absolute covariances of the 2nd degree moments of the joint density function:

$$\text{Cov}(x, y) = \iint (x - \langle x \rangle)(y - \langle y \rangle) f(x, y) dx dy \quad (2)$$

where $f(x, y)$ is the density function averaged over all variables other than x and y .

The total covariance matrix for a given energy-dependent cross-section (by isotope and type of reaction) is made up of the contribution of single covariance matrices, each one defining a type of correlation (between energy intervals or correlation with a different cross-section).

Review of the compilation, processing and analysis of uncertainty data for neutron induced reactions available in the most recent different internationally distributed nuclear data libraries has been performed for the purposes of the UAM LWR benchmark activities. The latest evaluated nuclear data files available from the OECD/NEA and NNDC-BNL are:

- 1) JENDL-3.3 (2002). The number of nuclides in this NDL is 337 and the covered incident neutron energy range is from 10^{-5} eV to 20 MeV. In JENDL-3.3, covariances are included for 20 nuclides. The physical quantities for which covariances are deduced are cross sections, resolved and unresolved resonance parameters, the first order Legendre-polynomial coefficient for the angular distribution of elastically scattered neutrons, and fission neutron spectra. Covariances were estimated on the basis of the same methods that were adopted in the JENDL-3.3 evaluation.
- 2) JEFF-3.1 (2005). The number of nuclides in this NDL is 381. The covariances are provided for 46 nuclides, and only for cross-sections. The latest version of the JEFF library, JEFF-3.1, was released by the NEA in May 2005.
- 3) ENDF/B-VI.8 (2001) and ENDF/B-VII.0 (2006). The later version of this NDL has 393 nuclides. The official version of ENDF/B-VII.0 was released at the end of 2006. The ENDF.B-VII library contains 14 sub-libraries (2 - new, 7 - many improvements and updates, 5 - unchanged). It is the largest library - it contains data for 393 materials (390 isotopes plus 3 elements). There are major improvements in the ENDF.B-VII library as compared to the previous versions/releases:

- Significant advances are made in evaluation of actinide cross-sections;
- Fission products are completely updated;
- Includes resonances (resolved and unresolved) in modern representation.

With regard to neutron cross section covariances (uncertainties plus correlation matrix) in the ENDF/B-VII library there is a drastic reduction compared to ENDF-B-VI.8 since the later covariances were from the 1970s and mostly produced for ENDF/B-V. It was decided to keep only quality covariances and 90 % of covariances were removed. Only partial covariances for 13 materials were migrated to ENDF/B-VII from ENDF/B-VI, and new covariances for 9 materials were added. The new covariances are for Gd isotopes, and this new evaluation includes unresolved resonances.

The covariance vision for the ENDF/B-VII as reported by BNL is as follows:

- Produce crude but reasonable covariances for all materials in ENDF/B-VII.0;
- Improve all covariances – and release VII.1 version (2010);
- Quality results – release VII.2 (2015).

When step a) is completed and made available it can be used for the purpose of the OECD LWR UAM benchmark. This will be low fidelity covariances and covariance matrix available for all materials in ENDF/B-VII.0 at any temperature, in a tabulated form or MF33 format. The delay in preparing the complete covariance data for the ENDF/B-VII is caused by the following reasons:

- Large multi-dimensional data representations are needed;
- Methods to evaluate the covariances are not well established;
- Covariance data for resonance parameters need special care.

The new BNL-LANL approach is utilized with covariances for the entire energy range: the fast neutron region is based on EMPIRE (BNL) [19, 20] and KALMAN (LANL) using both theoretical and experimental uncertainties, while the thermal and resonance regions are based on ATLAS (BNL) [21] and KALMAN. The SAMMY code (ORNL) [22, 23] will be used to generate resonance-parameter covariance matrices in the resolved and unresolved resonance regions for selected materials, while a simple “integral approximation” will be used to generate low fidelity uncertainties in the thermal and resonance ranges for most of the other materials. The “integral approximation” uses uncertainties in integral measurements of thermal cross sections and resonance integrals to approximate differential data uncertainties [24].

Table 1 shows the total number of materials and cross-section reactions with neutron cross-section covariance data in the recent versions of the major evaluated nuclear data files.

Table 1: Number of materials and cross-sections with covariances of neutron cross-sections

Data files	Number of materials	Number of cross-sections
ENDF/B-VI.8	44	400
JEFF-3.1	34	350
JENDL-3.3	20	160

The covariance data in the major data files is scarce in terms of materials (including actinides) and types of covariance matrices available. They contain uncertainty information only for few isotopes and reactions and usually for different number and different isotopes in different files. For isotopes not included, usually their covariances are assumed to be zero, which will result in the underestimation of core parameters uncertainties. For example the list of nuclides and materials present in LWR reactor cores of interest to this benchmark are given in Table 2z

through Table 4. These nuclides can be ranked according to their importance regarding the multiplication factor predictions. An example of such priority list of the most important nuclides for LWR calculations is given in

Table 5 (Please, note that the nuclides are not listed in the order of their importance.).

In conclusion, the status of presently available covariance data in the major NDLS is such that it can support only partially the objectives of the OECD LWR UAM benchmark. A first version of a more complete covariance data library is now ready containing low fidelity covariances that supplement available NDLS evaluations available for all required materials, it can be used for the purposes of this benchmark within the framework of Exercise I-1.

Table 2: Nuclides and materials present in TMI-1 PWR core calculations

H-1	B-10	B-11	C-0	O-16	Al-27	Si-0	Cr-0
Mn-0	Fe-0	Ni-0	Cu-63	Kr-83	Rh-103	Rh-105	Ag-107
Ag-109	Cd-113	In-115	I-135	Xe-131	Cs-133	Cs-134	Cs-135
Nd-143	Nd-145	Pm-147	Pm-148	Pm-148(m)	Pm-149	Sm-147	Sm-149
Sm-150	Sm-151	Sm-152	Eu-153	Eu-154	Eu-155	Gd-153	Gd-155
U-234	U-235	U-236	U-238	U-239	Np-237	Np-239	Pu-238
Pu-239	Pu-240	Pu-241	Pu-242	Am-241	Am-242(m)	Am-243	Cm-242
LFP1 ²	LFP2 ³	Zr-2 ⁴	Zr-4 ⁵	SS ⁶			

Table 3: Nuclides and materials present in PB-2 BWR core calculations

H-1	B-10	B-11	C-0	O-16	Kr-83	Rh-103	Rh-105
Ag-109	I-135	Xe-131	Xe-135	Cs-133	Cs-134	Cs-135	Nd-143
Nd-145	Nd-147	Pm-147	Pm-148	Pm-148(m)	Pm-149	Sm-147	Sm-148
Sm-149	Sm-150	Sm-151	Sm-152	Eu-153	Eu-154	Eu-155	Gd-154
Gd-155	Gd-156	Gd-157	Gd-158	Gd-160	U-234	U-235	U-236
U-238	U-239	Np-237	Np-239	Pu-238	Pu-239	Pu-240	Pu-241
Pu-242	Am-241	Am-242(m)	Am-243	Cm-242	Cm-244	Cm-245	Cm-246
Cm-247	LFP1	LFP2	Inc-718 ⁷	Zr-4	SS		

. These nuclides can be ranked according to their importance regarding the multiplication factor predictions. An example of such priority list of the most important nuclides for LWR calculations is given in

² Lumped fission products group 1

³ Lumped fission products group 2

⁴ Zircaloy-2

⁵ Zircaloy-4

⁶ Stainless Steel

⁷ Inconel-718

Table 5 (Please, note that the nuclides are not listed in the order of their importance.).

In conclusion, the status of presently available covariance data in the major NDLS is such that it can support only partially the objectives of the OECD LWR UAM benchmark. A first version of a more complete covariance data library is now ready containing low fidelity covariances that supplement available NDL evaluations available for all required materials, it can be used for the purposes of this benchmark within the framework of Exercise I-1.

Table 4: Nuclides and materials present in Kozloduy-6 VVER-1000 core calculations

H-1	B-10	B-11	C-0	N-14	O-16	Al-27	Si-0
P-31	S-0	Ti-0	Cr-0	Mn-55	Fe-0	Ni-0	Br-81
Kr-82	Kr-83	Kr-84	Kr-85	Kr-86	Sr-89	Sr-90	Y-89
Zr-0	Zr-91	Zr-93	Zr-95	Zr-96	Y-90	Nb-93	Nb-95
Mo-95	Mo-96	Mo-97	Mo-98	Mo-99	Mo-100	Tc-99	Ru-100
Ru-101	Ru-102	Ru-104	Ru-105	Ru-106	Rh-103	Rh-105	Pd-104
Pd-105	Pd-106	Pd-107	Pd-108	Ag-109	Ag-110(m)	Ag-111	Cd-110
Cd-111	Cd-113	In-115	Sb-0	Sb-125	Sb-127	Te-123	Te-127(m)
Te-129(m)	I-127	I-129	I-131	I-135	Xe-128	Xe-130	Xe-131
Xe-132	Xe-133	Xe-134	Xe-135	Xe-136	Cs-133	Cs-134	Cs-135
Cs-136	Cs-137	Ba-134	Ba-137	Ba-140	La-139	La-140	Ce-140
Ce-141	Ce-142	Ce-143	Ce-144	Pr-141	Pr-143	Nd-142	Nd-143
Nd-144	Nd-145	Nd-146	Nd-147	Nd-148	Nd-150	Pm-147	Pm-148
Pm-148(m)	Pm-149	Pm-151	Sm-147	Sm-148	Sm-149	Sm-150	Sm-151
Sm-152	Sm-153	Sm-154	Eu-151	Eu-153	Eu-154	Eu-155	Eu-156
Eu-157	Gd-154	Gd-155	Gd-156	Gd-157	Gd-158	Gd-160	Tb-159
Tb-160	Tb-161	Dy-160	Dy-160	Dy-161	Dy-162	Dy-164	Ho-165
Hf-174	Hf-176	Hf-177	Hf-178	Hf-179	Hf-180	Ta-181	Ta-182
U-235	U-236	U-237	U-238	Np-237	Pu-238	Pu-239	Pu-240
Pu-241	Pu-242	Am-241	Am-242(m)	Am-243	Cm-242	Cm-243	Cm-244
Cm-245	Cm-246	Cm-247	Cm-248	Bk-249	Cf-249	Cf-250	Cf-251
Cf-252							

Table 5: Priority list of important nuclides

H-1	B-10	B-11	O-16	Zr-91	Zr-93	Zr-96	Xe-136
Sm-149	Gd-155	Gd-157	U-234	U-235	U-236	U-237	U-238
Np-237	Np-239	Pu-238	Pu-239	Pu-240	Pu-241	Pu-242	Am-241
Am-242(m)	Am-243	Cm-242	Cm-244	Cm-245			

2.2 Multi-group processing of nuclear and covariance data

Prior to using the covariance information in applications, a processing method/code must be used to convert the energy-dependent covariance information to a multi-group format. Within the framework of Exercise I-1 the participants can use/develop their own processing methods or utilize available tools/codes at OECD/NEA and RSICC/ORNL to process the cross section data and associated covariance data (group-wise covariance matrices) for the multi-group libraries utilized as input in their lattice physics codes.

The data from the evaluated nuclear data files usually are processed with codes such as NJOY. The multi-group structures should correspond to the structure of input libraries in the utilized lattice physics codes. For example some of the input multi-group structures utilized for LWR analysis in lattice-physics codes are:

- a) CASMO-4 [25] input libraries – 40 and 70 groups;

- b) HELIOS [26] input libraries – 47 and 190 groups;
- c) APOLLO-2 [27] input libraries - 99 and 172 groups;
- d) TRITON [28] – 44 and 238 groups.

Uncertainties are inevitably introduced into the broad-group cross sections due to approximations in the grouping procedure. The dominant uncertainty is generally with regard to the energy weighting function used to average the point-wise or fine-group data within a single broad group. Intelligent choice of the weighting functions can reduce such uncertainties. Sensitivity studies using different group structures can help to identify uncertainties introduced with the choice of given multi-group structures. Multi-group library generation is as much an art as a science. Detailed knowledge of the specific application is needed to prepare adequately group constants. Continuous energy Monte Carlo solutions can be used to guide and inform multi-group library generation and use.

The SCALE system provides a rigorous mechanism for multi-group cross-section processing using the continuous energy solver CENTRM [29] for self-shielding in the resolved resonance and thermal regions for appropriately weighting multi-group cross-sections using a continuous-energy spectrum. The CENTRM module used for cross-section processing within SCALE performs an ultra-fine energy grid (typically 30,000-70,000 energy points) transport calculation using ENDF-based point data to generate effectively continuous energy neutron flux solutions in the resonance and thermal ranges. This is used to weight the multi-group cross-sections to be used in subsequent transport calculations. There is also a special sensitivity version of CENTRM that computes point-wise flux derivatives for evaluating implicit sensitivities associated with perturbations in resonance self-shielding.

The judicious selection of the energy group structure can also help to reduce the sensitivity of the computed responses to the weighting function, at least for a selected set of problems.

The covariance data can be processed in multi-group form. For example MF33 data are structured to be processed to yield the multi-group covariance matrices. There are several procedures to process covariances:

- a) ERRORR/COVR modules of NJOY [30] – can process ENDF Files 31, 32, 33 (not capable of processing Reich-Moore covariance data). Processed data are in COVFILS format.
- b) ERRORJ [31, 32] – can process the covariance for cross-sections including resonance parameters (Files 31, 32, 33, 34 and 35). It was recently integrated into the NJOY processing system. Processed data are generated in COVFILS format.
- c) PUFF-IV [33] – a multi-group covariance processing code. The PUFF-IV has the capability to process the uncertainty information in ENDF (Files 31, 32, 33) and generate the desired multi-group correlation matrix. Processed data are in COVERX format.
- d) SAMMY [34] - an R-matrix tool for analysis of cross section data in the resolved and unresolved resonance regions. SAMMY code can be used to generate a resonance-parameter covariance matrix in the resolved and unresolved resonance regions. The evaluated data files with covariance data are then processed with ERRORJ to generate multi-group covariance data for reactor applications. REFIT [35] is an alternative code to SAMMY with equivalent features.

In principle the covariance matrices can be now self-shielded in the same way as the cross-sections, although in practice this is rarely done. The impact of this treatment on the obtained covariance matrices and their dependence on energy group structure needs to be studied. The uncertainty can be self-shielded using Bondarenko factors, in the same way as the cross-sections are processed in the NJOY module GROUPR.

The ORNL's TSUNAMI system uses a completely different approach to address the impact of self-shielding in sensitivity analysis. Rather than modifying the covariance data, the sensitivity coefficients are modified to include the "implicit effects" of perturbations in the group cross sections caused by perturbations in self-shielding. Implicit effects account for impact of resonance self-shielding on sensitivity coefficients and uncertainty evaluations [36]. This allows the use of unshielded covariance data. Treatment of implicit effects is a standard part of the TSUNAMI analysis, and has been shown to be a significant sensitivity component in some cases [37].

Reducing the number of energy groups reduces the information contained in the covariance matrices. The point-wise cross-sections and associated Covariance Matrix (CM) are averaged using an energy dependent flux to give multi-group cross-sections and associated CM. The integrations used in the averaging process are usually evaluated using numerical integration schemes – any such schemes have an uncertainty associated with it.

Several multi-group covariance matrices have been developed and used for different applications. There are multi-group covariance matrices for major isotopes of interest in reactor core calculations based on a compilation of the available uncertainty data as shown in the Table 6:

- a) The multi-group ANL cross-section covariance matrix [38] was developed based on a simple "educated guess" for uncertainties and the simplest estimate for the correlation matrix. They found that the nuclear data uncertainties are significant for only a few parameters – k_{eff} for thermal systems at EOC due to high burnup; burnup reactivity swing and related isotopic density variations during core depletion. In the ANL covariance matrix the uncertainty values are given in an "energy band" consistent with multi-group structures used for deterministic calculations of both thermal and fast reactors. The ANL covariance matrix has been used with the ERANOS software based on generalized perturbation method for core calculations of GEN-IV design core models and very high burnup PWR core model.
- b) NEA covariance matrix is extracting relevant covariance data from current evaluations in major data files and processing them in a multi group structure. The name is NEA-1730: ZZ-COV-15GROUP. ZZ-COV-15GROUP is a 15-group (which can be expanded to a desired multi-group structure) cross section covariance matrix library presenting a general overview of the presently available data. The origin of this covariance matrix is from ENDF/B-V, /B-VI.8, JENDL-3.3, JEFF-3.0, IRDF-2002 and IAEA. It has been used with the cross-section sensitivity/uncertainty (S/U) SUS3D software available from OECD/NEA for propagation in core/experiment calculations.
- c) There are several evaluations of multi-group uncertainty libraries (44 groups) provided in the ORNL SCALE code package. These evaluations were generated by the multi-group preparation code PUFF-4, which processes the ENDF/B covariance data. These have been used by both TSUNAMI and TRITON. There are several different evaluations of multi-group uncertainty libraries (44 groups) provided in the ORNL SCALE code package. As it can be seen in Table 6 that the nuclide covariance data in SCALE 5.1 are the most complete – it is a collection of all covariance data produced over the last decades and critically reviewed for the most important nuclides. It is in 44 groups and can be expanded or reduced to the participants' multi-group structures. For these reasons it has been decided at the OECD UAM-1 workshop to utilize the nuclide multi-group covariance data in SCALE 5.1 for the purposes of Exercise I-1. The details of such utilization are given in Section 2.3.

History and description of SCALE covariance libraries are given below:

- a) The first covariance libraries were released in SCALE-5.0. These were the ones entitled, 44GROUPV5COV and 44GROUPANLCOV. They are now obsolete.
- b) In SCALE-5.1 the above covariance libraries were replaced by 4 COV libraries:
 - 44GROUPV5COV contains only covariances contained in ENDF/B-V;
 - 44GROUPV5REC contains ENDF/B-V covariances supplemented by other data sources (as described for 44GROUPV6REC below);
 - 44GROUPV6COV contains only covariances contained in ENDF/B-VI;
 - 44GROUPV6REC is the recommended covariance library based on several sources, including evaluated data files ENDF/B-VI, ENDF/B-V, JENDL, and JEF. Data missing from all evaluated data files were represented by the “integral approximation” described above, for the resonance and thermal energy ranges only. This approximation was used for approximately 300 materials.
- c) The SCALE-5.1 recommended covariance library is currently being updated to include recent high fidelity ENDF/B-VII uncertainty evaluations for the nuclides U-235, U-238, Pu-239, Th-232, and Gd isotopes. Some of the integral approximation data also is being revised to more recent measured values. This interim library should be available in January, 2008, and is being made available for the UAM effort. However it should be noted that the integral approximation for covariance data in the current library is incomplete at this time, since there are no values in the energy range above 5.5 keV. The final version of the new SCALE covariance library to be released in SCALE-6 during the latter part of 2008 should include a more complete set of uncertainties.

Table 6: Number of nuclides and energy groups in the available multi-group covariance matrices

Name	Number of nuclides	Number of energy groups
ANL	42	17
OECD/NEA	31	15
SCALE5.1/ORNL	299	44

2.3 Covariance data and tools distributed for the UAM Phase I project

The package distributed to UAM Phase I participants will consist of the following items distributed in 2 parts:

- 1) Cross-section relative covariance libraries:
 - a) A set of four cross-section covariance libraries [39] from the SCALE-5.1 [40] package and their documentation⁸. These libraries are in 44 energy groups in the original and the processed forms for user convenience.

⁸ These libraries have been released through the SCALE-5.1 package and are thus subject to US Export control. In order to obtain a copy, users must fill in the corresponding forms that can be obtained from the OECD/NEA Data Bank programs@nea.fr or directly from RSICC pdc@ornl.gov. Those who have a SCALE-5.1 license do not need a new license for these data.

- 2) Tools for handling and transforming the cross-section covariance data:
 - b) ANGELO – a code to transform these covariance data libraries into a user specified energy group-structure for the BOXR, COVFIL and COVERX formats [41, 42];
 - c) LAMBDA - a program for verifying the mathematical properties of the covariance data [41, 42].
- 3) In addition, it is recommended to use modules of the NJOY system (COVR) [30, 31] for plotting of the matrices and transformation to BOXR format. Utility routines of the ERRORJ [32] code package can be useful for COVERX files handling and conversion to COVFILS format (NJOY and ERRORJ can be obtained separately).

2.3.1 The cross-section relative covariance data sets

According to the SCALE 5.1 manual [39], “a total of four cross-section relative covariance libraries have been released:

- 44GROUPV5COV, Basic ENDF/B-V Covariance Library
- 44GROUPV5REC, Recommended ENDF/B-V Covariance Library
- 44GROUPV6COV, Basic ENDF/B-VI Covariance Library
- 44GROUPV6REC, Recommended ENDF/B-VI Covariance Library

These libraries correspond to the basic ENDF/B-V cross-section set, basic ENDF/B-VI set of cross sections, and two recommended sets that include the version V and VI sets plus a large number of nuclides for which covariance information is included, based on integral uncertainty data. Each of these sets contains cross-section covariance information in the SCALE 44 neutron energy group structure. It is envisaged to apply the covariance libraries to their respective ENDF/B-based cross-section libraries, (i.e., the V5 libraries to the version V cross-section libraries and the V6 libraries to the version VI cross-section libraries). In addition, there are two covariance sets for each ENDF/B version, corresponding to a *basic* set with only the materials included in the ENDF/B formal release and a *recommended* set with covariance information for most cross-section materials in the cross-section library. The *basic* sets do include substitutions and additions for nuclides with bad or missing covariance data such that they are useable in their present form. The *recommended* sets, while efforts were made to include covariance for every material, include most but not all of the materials present in the cross section library”.

In the report [39], tables are given with the missing data clearly identified. The files contain the covariance data for the following reactions or parameters: total, elastic, inelastic, (n,2n), fission, χ , (n, γ), (n,p), (n,d), (n,t), (n,³He), (n, α), and $\bar{\nu}$.

Table 7: The nuclides or materials (in ZA order) for which covariance data are provided

H-1(10)	H-2(3)	H-3(2)	He-3(2)	He-4	Li-6(2)	Li-7(3)	Be-9(2)
B-10(3)	B-11(2)	C-0(6)	N-14(2)	N-15	O-16(3)	O-17	F-19(3)
Na-23(3)	Mg-0	Al-27(2)	Si-0(3)	Si-28	Si-29	Si-29	Si-30
P-31	S-0	S-32	Cl-0	K-0	Ca-0	Sc-45(2)	Ti-0
V-0(2)	Cr-0(2)	Cr-50	Cr-52	Cr-53	Cr-54	Mn-55(3)	Fe-0(2)
Fe-54	Fe-56	Fe-57	Fe-58	Co-59(3)	Ni-0(2)	Ni-58	Ni-60
Ni-61	Ni-62	Ni-64	Cu-0	Cu-63	Cu-65	Ga-0	Ge-72
Ge-73	Ge-74	Ge-76	As-75	Se-74	Se-76	Se-77	Se-78
Se-80	Se-82	Br-79	Br-81	Kr-78	Kr-80	Kr-82	Kr-83
Kr-84	Kr-85	Kr-86	Rb-85	Rb-87	Sr-84	Sr-86	Sr-87
Sr-88	Sr-89	Sr-90	Y-89	Y-89	Y-90	Y-91	Zr-0
Zr-90	Zr-91	Zr-92	Zr-93	Zr-94	Zr-96	Nb-93	Nb-93
Nb-94	Nb-95	Mo-0	Mo-94	Mo-95	Mo-96	Mo-97	Tc-99
Ru-96	Ru-99	Ru-100	Ru-101	Ru-102	Ru-104	Ru-105	Ru-106
Rh-103	Rh-105	Pd-102	Pd-104	Pd-105	Pd-106	Pd-107	Pd-108
Pd-110	Ag-107	Ag-109	Ag-111	Cd-0	Cd-106	Cd-108	Cd-110
Cd-111	Cd-112	Cd-113	Cd-114	Cd-116	In-0	In-113	In-115
Sn-112	Sn-114	Sn-115	Sn-116	Sn-117	Sn-118	Sn-119	Sn-120
Sn-122	Sn-124	Sb-121	Sb-123	Sb-124	Te-120	Te-122	Te-123
Te-124	Te-125	Te-126	Te-127(m)	Te-128	Te-130	I-127	I-129
I-130	I-131	Xe-124	Xe-126	Xe-128	Xe-129	Xe-130	Xe-131
Xe-132	Xe-133	Xe-134	Xe-135	Xe-136	Cs-133	Cs-134	Cs-135
Cs-137	Ba-134	Ba-135	Ba-136	Ba-137	Ba-138	Ba-140	La-139
La-140	Ce-140	Ce-141	Ce-142	Ce-143	Ce-144	Pr-141	Pr-142
Pr-143	Nd-142	Nd-143	Nd-144	Nd-145	Nd-146	Nd-147	Nd-148
Nd-150	Pm-147	Pm-148	Pm-148(m)	Pm-149	Sm-144	Sm-147	Sm-148
Sm-149	Sm-150	Sm-151	Sm-152	Sm-153	Sm-154	Eu-151	Eu-152
Eu-153	Eu-154	Eu-155	Gd-152	Gd-154	Gd-155	Gd-156	Gd-157
Gd-158	Gd-160	Tb-159	Tb-160	Dy-160	Dy-161	Dy-162	Dy-163
Dy-164	Ho-165	Er-166	Er-167	Lu-175	Lu-176	Hf-0	Hf-174
Hf-176	Hf-177	Hf-178	Hf-179	Hf-180	Ta-181	Ta-182	W-0
W-182	W-183	W-184	W-186	Re-185(2)	Re-187(2)	Au-197(3)	Pb-0(2)
Pb-206	Pb-207	Pb-208	Bi-209(2)	Th-230	Th-232(4)	Pa-231	Pa-233(3)
U-232	U-233	U-234	U-235	U-235(6)	U-236	U-237	U-238(4)
Np-237(2)	Pu-0	Pu-238(7)	Pu-239(9)	Pu-240(10)	Pu-241(11)	Pu-242(3)	Pu-243
Pu-244	Am-241(4)	Am-242	Am-242(m)	Am-243	Cm-242	Cm-243	Cm-244
Cm-245	Cm-246	Cm-247	Cm-248	Bk-249	Cf-249	Cf-250	Cf-251
Cf-252(3)	Cf-253	Es-253					

In parentheses the total number of the different relative covariance matrices in the four libraries for each nuclide is specified. In Appendices I through IV the list of nuclides and the origin of the covariance data are provided for each library. The 44 energy-groups structure is described in Appendix V.

Some of the covariance data covers only the thermal and resonance region (based on Mughabghab (BNL) thermal and resonance integral uncertainty evaluation – this represents a large fraction of the covariance data). It is a collection of all covariance data produced over the last decades in which the most important nuclides have been critically reviewed.

These libraries will be delivered in the original SCALE COVERX format. A slightly modified routine EDITCVX from the code ERRORJ [32] was used to subdivide the original libraries into separate COVERX format files for each nuclide or material. This allows ‘cleaning up’ the files removing zero covariances, and in particular easier handling and faster ANGELO runs. Although it is in principle possible to process both the

original as well as the separated COVERX files with the ANGELO and LAMBDA codes, the use of separate files is recommended.

Following a request from the UAM (Uncertainty Analysis in Modeling) expert group, the authorization was granted by the SCALE management and DOE to use the group cross-section covariance data now distributed with SCALE-5.1 for the purpose of the Phase I (Neutronics Phase) benchmark study and in connection with other codes.

2.3.2 Tools for handling and transforming the cross-section relative covariance data

The code ANGELO [41, 42] is designed for the interpolation of the multi-group covariance matrices from the original to a user defined energy structure which is also distributed for the convenience of the users. The algorithm used in the ANGELO code is relatively simple; therefore the interpolations involving the energy group structures which are very different from the original one (such as large difference in the number of energy groups) are to be avoided as they may not be accurate. ANGELO does not carry out cross-section and flux weighting; therefore the interpolations to group structures which differ significantly from the original should be avoided (especially if the number of groups is reduced considerably). Still, the procedure tends to be conservative. The interpolation procedure was found to give reliable results if the number of groups changed by up to a factor of 4. In this range the procedure can therefore be considered as an adequate and easy-to-use alternative to more rigorous methods, like the ERRORR module of NJOY. Several input formats are available for the covariance files: BOXR, COVERX and several flexible text file formats. The output format is COVFILS (recommended) and different binary formats. The COVFILS format is native of NJOY [30, 31] which allows using the NJOY module COVR to perform covariance plotting and output formatting operations, such as transformation to the compact BOXR format. The utility programs of ERRORJ can be also used to convert COVFILS format to COVERX. The input description is provided as Appendix VI.

LAMBDA [41, 42] is a program to verify some mathematical properties and the physical consistency of the data and the interpolation procedure, in particular the positive definiteness of the multigroup covariance matrices. The trace and the number of positive, negative, and zero eigenvalues are calculated and the matrix is classified on this basis. The correlation matrix is tested to determine if any element exceeds unity. This quality verification is highly recommended before using the covariance information to data consistency analyses with integral experiments and to data adjustment. Accepted input formats are BOXR and COVERX. The input description is provided in Appendix VI.

2.4 Test problems

The uncertainty files (nuclear data uncertainties) in the evaluated NDLs are obtained from the analysis of experimental differential data and from nuclear models and are stored as variance and covariance data. Within the framework of Exercise I-1 the cross-section uncertainty data is processed in a multi-group format. The final multi-group cross-section libraries and associated uncertainties should be consistent with requirements of lattice physics codes, which participants are planning to utilize. In order to perform a comparative analysis of the multi-group cross-section uncertainty data obtained after processing test problems are devised or utilized from the previously defined benchmarks (participants can select which test problem to analyze and submit results for):

- 1) Two-dimensional fuel pin-cell test problems representative of BWR PB-2 [6], PWR TMI-1 [7], and Kozloduy-6 VVER-1000 [8].

The specifications of these three test problems are given subsequently in Figure 1 through Figure 3. The figures include geometry and material specifications. The reflective boundary conditions are utilized at the boundaries of problems. These problems have to be analyzed at Hot Zero Power (HZP) conditions as defined in the Table 8:

Table 8: HZP conditions for LWR fuel pin-cell test problems

HZP Conditions / Reactor	PB-2 BWR	TMI-1 PWR	Kozloduy-6 VVER-1000
Fuel and Moderator (Coolant) Temperatures, °K	552.833	551.000	552.150
Moderator (Coolant) Density, kg/m ³	753.978	766.000	767.100
Reactor Power, MW	3.293	2.772	3.000

First, one group effective uncertainties will be compared. The effective uncertainties have to be obtained by each participant using his/her multi-group uncertainty data associated with the multi-group library used as input in his/her lattice physics code. The effective uncertainty (relative error) for neutron cross-sections corresponding to the neutron flux spectrum of the pin-cell test problem of interest can be obtained as follows:

$$\Delta^2 = \sum_{\substack{i \in n \\ j \in n}} \alpha_i \cdot \text{cov}(i, j) \cdot \alpha_j \quad (3)$$

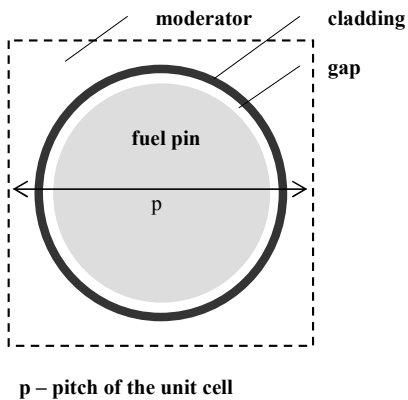
where:

$$\alpha_j = \frac{\bar{\sigma}_i^{eff}}{\bar{\sigma}} = \frac{\bar{\sigma}_i \bar{\phi}_i}{\bar{\sigma} \bar{\phi}_T};$$

ϕ_i is the multi-group neutron flux;

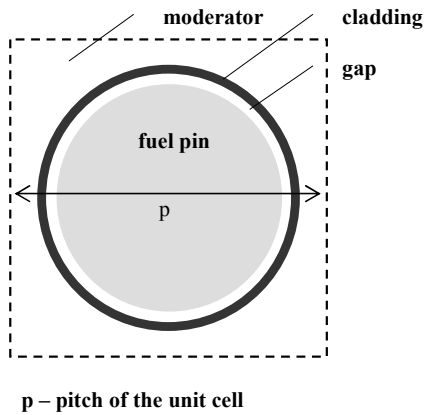
$$\phi_T = \sum_{i \in n} \phi_i \text{ with } n \text{ the total number of energy groups;}$$

$\text{cov}(i, j)$ is the ENDF multi-group covariance matrix.



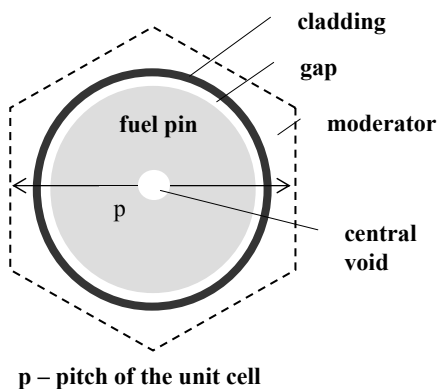
Parameter	Value
Unit cell pitch, mm	18.75
Fuel pellet diameter, mm	12.1158
Fuel pellet material	UO ₂
Fuel density, g/cm ³	10.42
Fuel enrichment, w/o	2.93
Cladding outside diameter, mm	14.3002
Cladding thickness, mm	0.9398
Cladding material	Zircaloy-2
Gap material	He
Moderator material	H ₂ O

Figure 1: Configuration of PB-2 BWR unit cell



Parameter	Value
Unit cell pitch, mm	14.427
Fuel pellet diameter, mm	9.391
Fuel pellet material	UO ₂
Fuel density (95% TD), g/cm ³	10.283
Fuel enrichment, w/o	4.85
Cladding outside diameter, mm	10.928
Cladding thickness, mm	0.673
Cladding material	Zircaloy-4
Gap material	He
Moderator material	H ₂ O

Figure 2: Configuration of TMI-1 PWR unit cell



Parameter	Value
Unit cell pitch, mm	12.75
Fuel pellet diameter, mm	7.56
Fuel pellet material	UO ₂
Fuel density, g/cm ³	10.4
Fuel enrichment, w/o	3.3
Central void diameter, mm	1.4
Central void material	air
Cladding outside diameter, mm	9.1
Cladding thickness, mm	0.69
Cladding material	Zr +1% Nb
Gap material	He
Moderator material	H ₂ O

Figure 3: Configuration of Kozloduy-6 VVER unit cell

These effective uncertainties have to be calculated for the neutron cross-sections of the nuclides present in the pin-cell models.

In addition, for each test problem participants have to calculate k_{inf} , and absorption and fission reaction rates for ^{234}U , ^{235}U , and ^{238}U and associated uncertainties due to multi-group cross-sections based on the multi-group covariance matrices processed in Exercise I-1.

- 2) Fuel pin-cell test problems from the KRITZ-2 LEU critical experiments [43, 44]. The KRITZ-2:1 and KRITZ-2:13 experiments at two different temperatures and boron concentration are selected for the purposes of the OECD LWR UAM benchmark since their rod pitch sizes are similar to those of lattices present in the PB-2 and TMI-1 cores. For each test problem and case participants have to calculate k_{inf} , and absorption and fission reaction rates for ^{234}U , ^{235}U , and ^{238}U and associated uncertainties due to multi-group cross-sections based on the multi-group covariance matrices processed in Exercise I-1.
- 3) It is well known that the available clean core measurements at facilities for thermal systems can be used to assess the performance of nuclear data libraries. That is why the critical configurations (core) test problems from the above-mentioned KRITZ-2 LEU critical experiments - KRITZ-2:1 and KRITZ-2:13 (for which measured data is available) – are also utilized. For each problem the participants have to calculate the configuration multiplication factors (k_{eff}) at “room” and “elevated” temperatures and the relative rod powers for the rods for which the measurements were performed as well as associated uncertainties due to multi-group cross-sections based on the multi-group covariance matrices processed in Exercise I-1. By including the uncertainty or covariance information, the analyst can propagate cross-section data uncertainties through sensitivity studies to the final calculated quantities of interest and compare with the measurement uncertainty.
- 4) VVER physics experiments [44⁹, 52¹⁰] performed at the critical facility of the Russian Research Center “Kurchatov Institute” (RRC KI) are selected for the purposes of the OECD LWR UAM benchmark since their rod pitch sizes are similar to those of lattices present in the Kozloduy-6 and Kalinin-3 cores. These experiments were carried out using light water fuel lattices of VVER 1000 fuel assemblies. Cases 1, 2, and 9 are selected to be simulated. For each case the participants have to calculate the configuration multiplication factors (k_{eff}) at “room” temperature and associated uncertainties. For case 9 the relative radial fission reaction rate distribution and associated uncertainties have to be calculated.

The KRITZ and VVER experimental test problems are also designed as 2-D problems, which utilized experimental axial bucklings to be used for accounting of the axial leakage. Continuous-energy Monte Carlo (MCNP5) solutions with converged eigenvalue and fission source distribution will be provided for each test problem. The statistical uncertainties in the reference Monte Carlo calculations will be evaluated by the benchmark team. In the calculations of the above-described test problems the participants have to utilize their multi-group cross-section libraries (input to their lattice physics codes) and associated uncertainties. They can utilize their own Sensitivity/Uncertainty (S/U) tools to propagate cross-section uncertainties to calculate quantities of interest in nuclear analysis or the ones available at OECD/NEA – such as SUS3D [45] – and ORNL – such as TSUNAMI [37].

The objective of Exercise I-1 is to address the uncertainties due to the basic nuclear data as well the impact of processing the nuclear and covariance data. Within Exercise I-1 the uncertainties in evaluated NDIs are

⁹ PFacility-VVER-EXP-001

¹⁰ LEU-COMP-THERM-061

propagated into multi-group microscopic cross-sections used as an input by their lattice physics codes. The output uncertainties of Exercise I-1 are input uncertainties in Exercise I-2.

Chapter 3

DEFINITION OF EXERCISE I-2: LATTICE PHYSICS

This exercise includes the propagation of input uncertainties, defined below, through lattice physics calculations to output uncertainties in evaluated lattice-averaged (homogenized assembly/node) parameters e.g. few-group homogenized nodal parameters such as cross-sections, assembly discontinuity factors, form functions and k_{inf} . The input uncertainties, which result in uncertainties in prediction of lattice-averaged parameters and which need to be accounted for and propagated, are arising from:

- Multi-group cross-section uncertainties (multi-group cross-section covariance matrix);
- Uncertainties associated with methods and modeling approximations utilized in lattice physics codes;
- Fuel/assembly manufacturing uncertainties.

In order to propagate the input uncertainties through lattice physics calculations to determine uncertainties in output lattice-averaged parameters within the framework of Exercise I-2 the utilization of a lattice physics code is necessary. Participants can use/select their own lattice physics codes in conjunction with their own UA and SA tools for the purposes of this exercise.

3.1 Discussion of input and target (output) uncertainties

In the current established calculation scheme for LWR design and safety analysis, multi-group microscopic cross-section libraries are an input to lattice physics calculations. The multi-group cross-section uncertainties (multi-group cross-section covariance matrix) should be obtained by participants as output uncertainties within the framework of Exercise I-1. In Exercise I-2 multi-group cross-section uncertainties are input uncertainties and must be propagated through the lattice physics calculations to few-group cross-section uncertainties (few-group covariance matrix). All cross-section uncertainties are assumed to follow normal Gaussian distributions and only the first and second moments of the uncertainty distributions i.e. the means and covariances, are to be propagated through the calculations [46, 47]. The propagation of the cross-section uncertainties is the most important part of Exercise I-2.

The other input uncertainties in Exercises I-2 are new uncertainties added during the cross-section generation process. Methodological uncertainties, which are associated with methods and modeling approximations utilized in lattice physics codes, should be assessed. Different transport methods have been utilized in lattice physics codes such Collision Probabilities Method (CPM), Method of Characteristics (MOC), S_n , P_n and etc. Depending on the availability of different methods in the lattice code of choice, the related uncertainties can play a smaller or larger role. The participants are responsible of performing spatial discretization and angular discretization convergence studies with their lattice physics codes in order to remove the uncertainties associated with numerical approximations (numerical method uncertainties) and reduce the uncertainties associated with neutron transport method (physics uncertainties) used in lattice physics codes. The method related contribution of uncertainty can be derived from earlier benchmarks conducted within OECD/NEA.

In the current LWR standard calculation scheme (utilized in industry and regulation) the lattice physics calculations for generation of few-group cross-sections usually the following approximations (on which participant should focus as a second important input uncertainty apply):

- a) Pin cell homogenization;
- b) Energy group condensation;
- c) Assembly homogenization in single assembly environment.

In order to assess the uncertainties in few-group assembly homogenized cross-sections and other nodal homogenized parameters (Assembly Discontinuity Factors – ADFs, Corner Discontinuity Factors – CDFs, Form Functions) due to utilization of the above-mentioned approximations, one has to decompose and evaluate the errors of these approximations. Evaluation of the uncertainties introduced with such modeling approximations is important because in some situations these approximations work well and in others they do not. This can be accomplished by designing appropriate 2-D mini-core test problems (color-sets) [48] in addition to 2-D single assembly models with reflective boundary conditions. The latter are the base models for cross-section generation with the exception of reflector cross-sections, which are usually generated in 1-D color-sets. For this reason, 2-D color-set test problems are defined by the benchmark team for this Exercise in addition to the single assembly and 1-D color-set models.

The participants should also account for fuel/assembly manufacturing uncertainties such as enrichment, pellet density, cladding dimensions, BP concentration, and assembly geometry. Assignment of uncertainty measures in the form of PDFs to all input variables should be considered. For example for the PDFs for pellet dimensions, density, Zr homogenization for the pin cell, and initial isotopic content can be assumed as normal distribution [49]. The benchmark team will provide to participants the ranges of changes and PDFs associated with the fuel/assembly manufacturing uncertainties for the different test problems as described below.

3.2 Test problems

Different stand-alone neutronics single assembly and mini-core test problems have been designed for the purposes of the Exercise I-2 utilizing information from the previous OECD coupled code benchmarks - BWR PB-2 [6], PWR TMI-1 [7], and Kozloduy-6 VVER-1000 [8].

- 1) 2-D assembly model with reflective boundary conditions. This is the standard model utilized for fuel assembly cross-section generation in LWR analysis.

The information for the BWR single assembly model is given in Table 9 and Figure 4. The information for the PWR single assembly model is given in Table 10 and Figure 10. The information for the VVER single assembly model is given in Table 12 and Figure 14. These problems have to be analyzed at Hot Zero Power (HZP) conditions as defined in the Table 8.

First, one group effective uncertainties will be compared. The effective uncertainties have to be obtained from each participant using his/her few-group uncertainty data (obtained few-group covariance matrix) associated with the few-group cross-section data. The effective uncertainty (relative error) for few-group neutron cross-sections corresponding to few-group neutron flux spectrum of the single assembly test problem of interest can be obtained using formulae (3) in Section 2.4.

Second, a comparison of uncertainties in two-group structure will be performed. Participants have to obtain them from the few-group covariance matrices derived within Exercise I-2 for the assembly

model of interest and provide them. The output uncertainties of the following few-group assembly homogenized parameters will be compared:

- a) k_{inf} , absorption and fission reaction rates, and associated uncertainties;
 - b) ADFs, CDFs, Form Functions;
 - c) Kinetics and delayed neutron parameters.
- 2) 1-D assembly/reflector model (color set) with reflective boundary conditions on the left boundary and vacuum boundary condition on the right boundary. This is the standard model utilized for reflector cross-section generation in LWR analysis.

The information for the BWR model is given in Figure 9. The information for the PWR model is given in Figure 13. The information for the VVER model is given Figure 17. These problems have to be analyzed at Hot Zero Power (HZP) conditions as defined in the Table 8.

The output uncertainties of the following few group reflector homogenized parameters will be compared: macroscopic cross-sections of different reactions and ADFs.

- 3) 2-D assembly color sets (mini-cores). Different mini-core problems were developed involving unrodded, rodded and reflector assemblies. For mini-cores without reflector reflective boundary conditions are utilized. For mini-cores with reflector zero-flux boundary conditions are utilized.

The information for BWR mini-cores is given in Figure 7 and Figure 8. The information for PWR mini-cores is given in Table 11 and Figure 11 and Figure 12. The information for VVER mini-cores is given in Figure 15 and Figure 16. These problems have to be analyzed at Hot Zero Power (HZP) conditions as defined in the Table 8.

For each problem the participants have to calculate the mini-core multiplication factors (k_{eff}) and the relative pin powers as well as associated uncertainties due to the few-group cross-section generation process within Exercise I-2.

Continuous Monte Carlo (MCNP5) solutions with sufficient statistics to assure not only k_{inf} (k_{eff}) but also fission source convergence will be used as reference solutions for the single assembly and different color-set test problems designed for Exercise I-2. The statistical uncertainties in the reference Monte Carlo calculations will be evaluated by the benchmark team.

Exercise I-2 propagates input uncertainties obtained from Exercise I-1 and other input uncertainties added in Exercise I-2. The objective of Exercise I-2 is to obtain uncertainty estimates of k_{inf} , and few group homogenized parameters used in core calculations as a function of the uncertainties discussed above.

The output uncertainty of Exercise I-2 is propagated in Exercises I-3, II-3, III-1 and III-3. The major effort is focused on obtaining uncertainties in two group homogenized parameters. Provision for few group (more than two energy group) homogenized parameters and associated uncertainties with selected by participants few-group structures is made.

Table 9: PB-2 fuel assembly data

	Initial load			Reload	Reload	LTA special
Assembly type	1	2	3	4	5	6
No. of assemblies, initial core	168	263	333	0	0	0
No. of assemblies, Cycle 2	0	261	315	68	116	4
Geometry	7 × 7	7 × 7	7 × 7	8 × 8	8 × 8	8 × 8
Assembly pitch, mm	152.4	152.4	152.4	152.4	152.4	152.4
Fuel rod pitch, mm	18.75	18.75	18.75	16.23	16.23	16.23
Fuel rods per assembly	49	49	49	63	63	62
Water rods per assembly	0	0	0	1	1	2
Burnable poison positions	0	4	5	5	5	5
No. of spacer grids	7	7	7	7	7	7
Inconel per grid, kg	0.225	0.225	0.225	0.225	0.225	0.225
Zr-4 per grid, kg	1.183	1.183	1.183	1.353	1.353	1.353
Spacer width, cm	4.128	4.128	4.128	4.128	4.128	4.128
Assembly average fuel composition:						
Gd ₂ O ₃ , g	0	441	547	490	328	313
UO ₂ , kg	222.44	212.21	212.06	207.78	208.0	207.14
Total fuel, kg	222.44	212.65	212.61	208.27	208.33	207.45

Rod type	Number of rods	Pellet density		Stack density (g/cm ³)	Gd ₂ O ₃ (g)	UO ₂ (g)	Stack length (cm)
		UO ₂ (g/cm ³)	UO ₂ +Gd ₂ O ₃ (g/cm ³)				
1	25	10.42	–	10.32	0	4 352	365.76
1s	1	10.42	–	10.32	0	3 935	330.20
2	12	10.42	–	10.32	0	4 352	365.76
3	6	10.42	–	10.32	0	4 352	365.76
4	1	10.42	–	10.32	0	4 352	365.76
5A	3	–	10.29	10.19	129	4 171	365.76
6B	1	10.42	10.29	10.27	54	4 277	365.76

Pellet outer diameter = 1.21158 cm.

Cladding = Zircaloy-2, 1.43002 cm outer diameter × .09398 cm wall thickness, all rods.

Gas plenum length = 40.132 cm.

Assembly design for Type 2 initial fuel

Rod type	²³⁵ U (wt.%)	Gd ₂ O ₃ (wt.%)	No. of rods
1	2.93	0	26
2	1.94	0	12
3	1.69	0	6
4	1.33	0	1
5A	2.93	3.0	3
6B	2.93	3.0	1

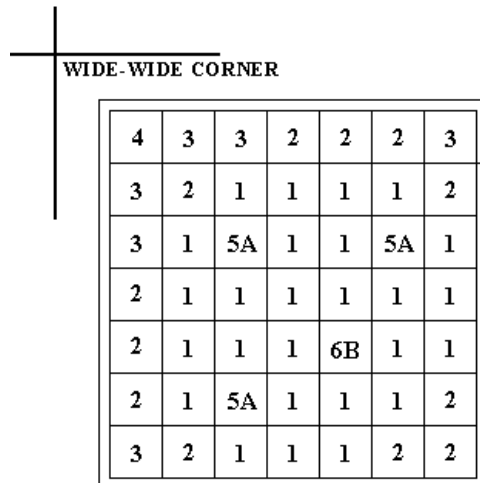
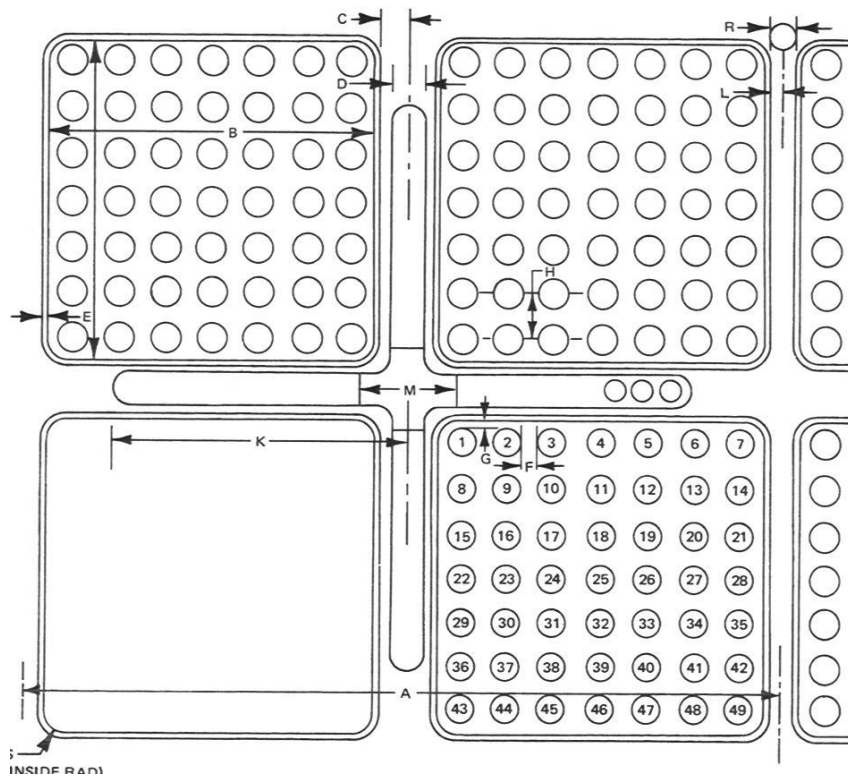


Figure 4: PB-2 assembly design - Type 2 initial fuel



Dim. ID	A	B	C	D	E	F	G	H	I	J
Dim. (cm)	30.48	13.40612	0.9525		0.2032	0.4445	0.36449	1.87452		
Dim. ID	K	L	M	N	O	P	Q	R	S	
Dim. (cm)		0.47498							0.9652	

Figure 5: PB-2 initial fuel assembly lattice (Type 2)

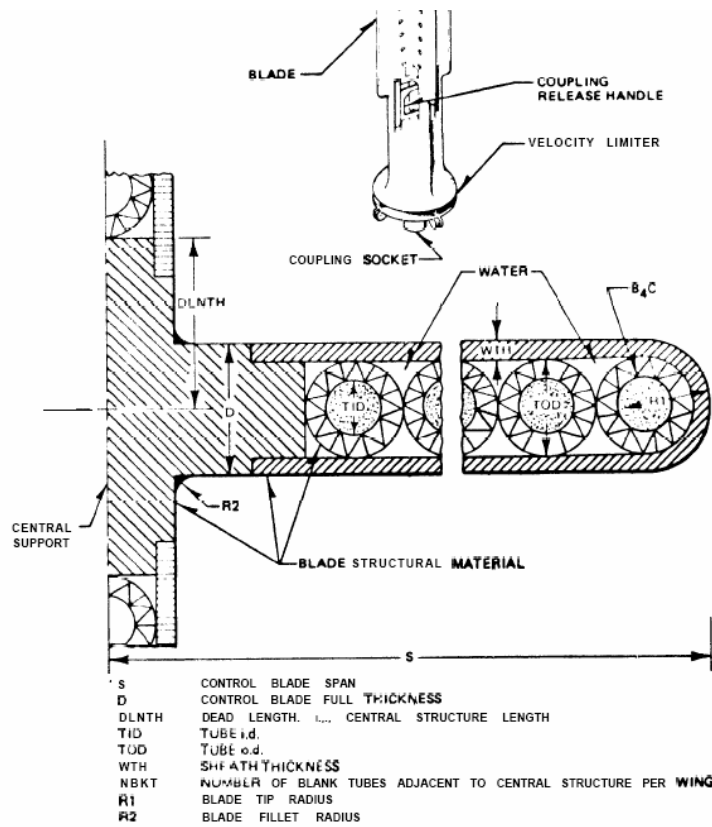


Figure 22. B₄C Control Blade Model (Schematic)

Shape	Cruciform
Pitch, cm	30.48
Stroke, cm	365.76
Control Length, cm	363.22
Control Material	B ₄ C granules in Type-304 stainless steel tubes and sheath
Material Density	70% of theoretical (2.52 g/cm ³)
Number of Control Material	
Tubes per Rod	84
Tube Dimensions	0.47752 cm OD by 0.0635 cm wall
Control Blade Half Span, cm	12.3825
Control Blade Full Thickness, cm	0.7925
Control Blade Tip Radius, cm	0.39624
Sheath Thickness, cm	0.14224
Central Structure Wing Length, cm	1.98501
Blank tubes per wing	none

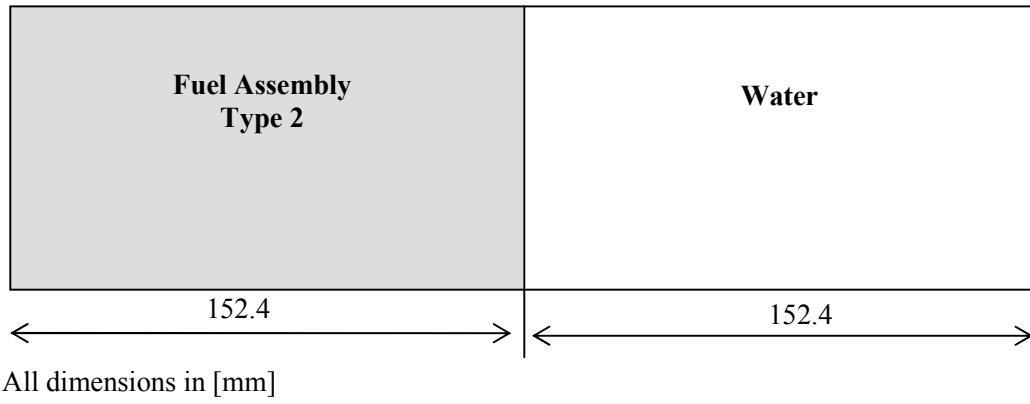
Figure 6: Control rod blade model and characteristics for PB-2

rodded	unrodded
unrodded	rodded

Figure 7: Color-set configuration for PB-2

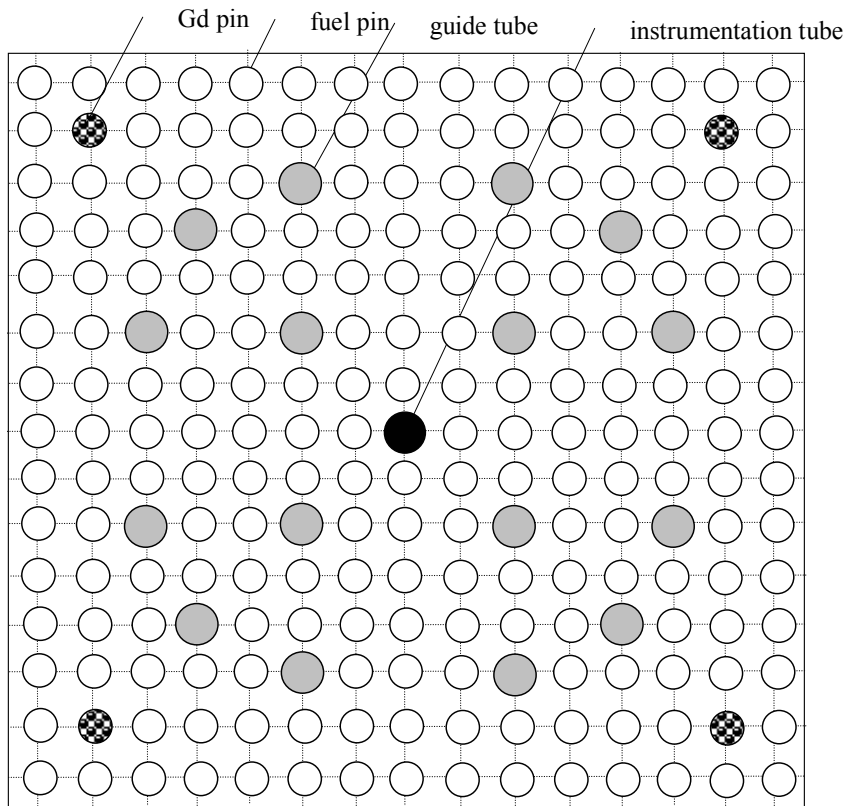
reflector	reflector	reflector	reflector	reflector	reflector	reflector	reflector
reflector	unrodded	unrodded	unrodded	unrodded	unrodded	unrodded	reflector
reflector	unrodded	unrodded	unrodded	unrodded	unrodded	unrodded	reflector
reflector	unrodded	unrodded	rodded	rodded	unrodded	unrodded	reflector
reflector	unrodded	unrodded	rodded	rodded	unrodded	unrodded	reflector
reflector	unrodded	unrodded	unrodded	unrodded	unrodded	unrodded	reflector
reflector	unrodded	unrodded	unrodded	unrodded	unrodded	unrodded	reflector
reflector	reflector	reflector	reflector	reflector	reflector	reflector	reflector

Figure 8: Color-set configuration for PB-2 (with reflector)



Reflector Material	Composition
Water (H ₂ O)	H - 11.19 % ; O - 88.81 %

Figure 9: PB-2 radial reflector model – dimensions and material compositions



Parameter	Value
Fuel assembly dimensions	15 × 15
Number of fuel rods per FA	208
Number of guide tubes per FA	16
Number of instrumentation tubes per FA	1
Number of Gd pins per FA	4
Fuel rod pitch, mm	14.427
Fuel rod outside diameter, mm	10.922
Fuel pellet diameter, mm	9.390
Cladding thickness, mm	0.673
Guide tube outside diameter, mm	13.462
Guide tube inside diameter, mm	12.649
Instrumentation tube outside diameter, mm	12.522
Instrumentation tube inside diameter, mm	11.201
Fuel assembly pitch, mm	218.110
Gap between fuel assemblies, mm	1.702

Figure 10: TMI-1 assembly design

Table 10: TMI-1 assembly material compositions

Material	Composition
Spacer grids	Zircaloy-4
Central tube	Zircaloy -4
Guide tubes	Zircaloy -4

Table 11: TMI-1 control rod assembly data

Item	Data
Number of control rods per assembly	16
Outside diameter of control rod, mm	11.2014
Cladding thickness, mm	0.5715
Cladding material	Inconel 625
Absorber material	Ag - 80 %, In - 15%, Cd - 5%
Length of absorber section, mm	3530.6

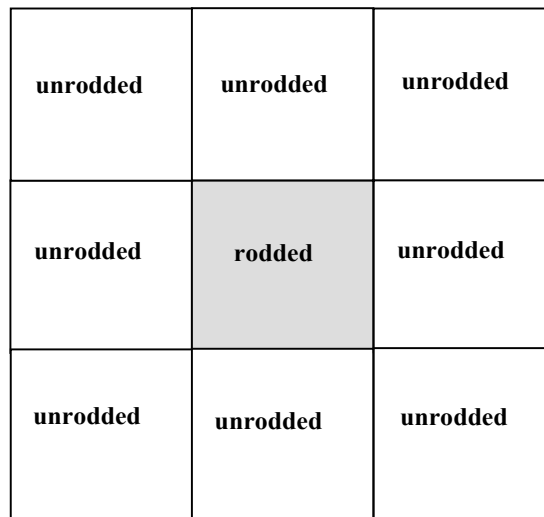


Figure 11: Color-set configuration for TMI-1

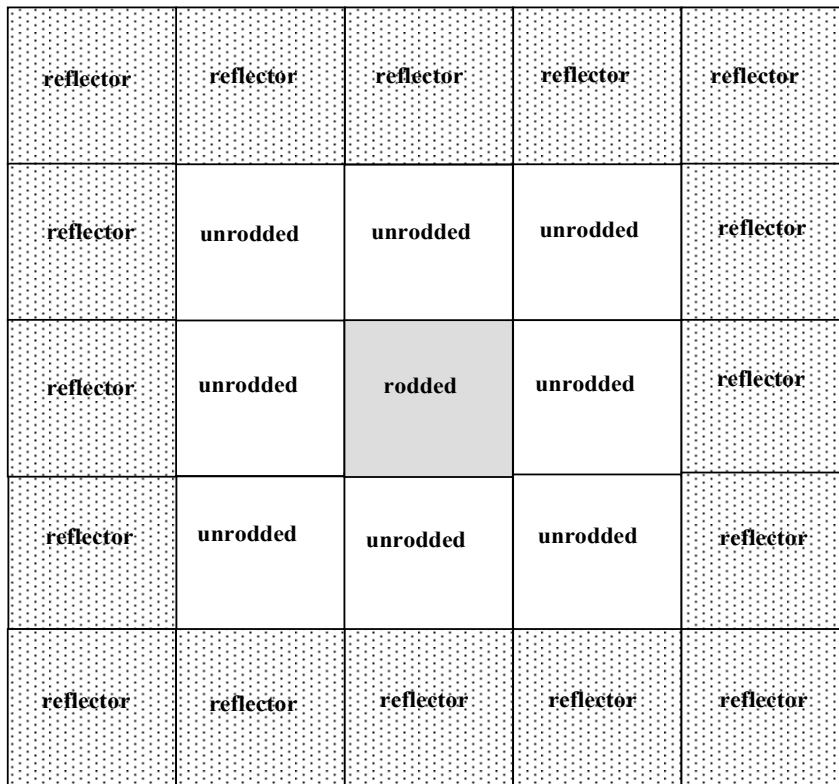
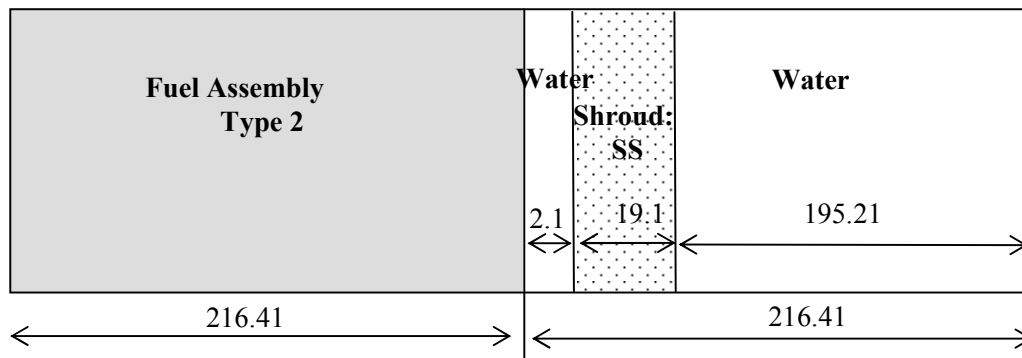


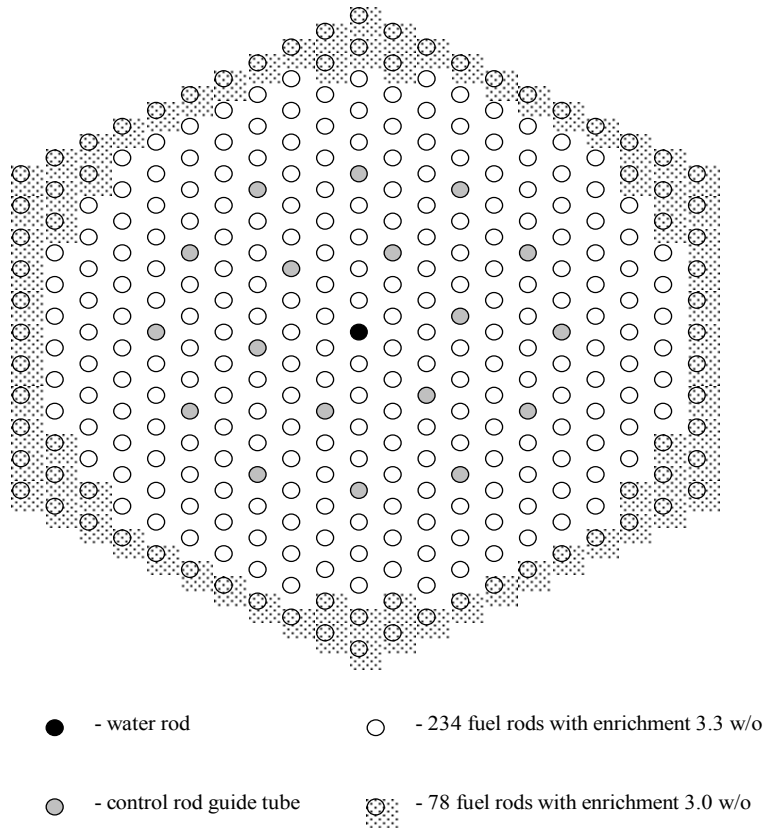
Figure 12: Color-set configuration for TMI-1 (with reflector)



All dimensions in [mm]

Material	Composition
Water (H ₂ O)	H - 11.19 % ; O - 88.81 %
Shroud (SS)	Stainless steel

Figure 13: TMI radial reflector model – dimensions and material compositions

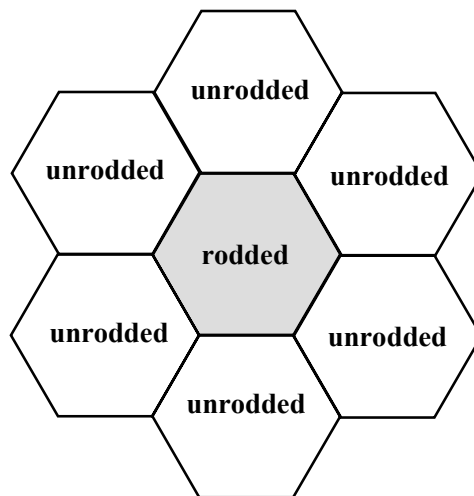


Parameter	Value
Number of fuel rods	312
Number of fuel rods with 3.0 w/o enrichment	78
Number of fuel rods with 3.3 w/o enrichment	234
Number of water rods per FA	1
Number of guide tubes	18
Pellet diameter, mm	7.56
Central void diameter, mm	1.4
Cladding outside diameter, mm	9.1
Cladding thickness, mm	0.69
Fuel rods pitch, mm	12.75
Guide tube outside diameter, mm	12.6
Guide tube inside diameter, mm	11.0
Absorber (control rods) pellet diameter, mm	7.0
Absorber cladding outside diameter, mm	8.2
Water rod outside diameter, mm	11.2
Water rod inside diameter, mm	9.6

Figure 14: Kozloduy-6 assembly design

Table 12: Kozloduy-6 assembly material compositions

Material	Composition
Spacer grids : Steel 08X18H10T; 1.2 % of the FA volume	C - 0.08%, Si-0.8%, Mn-2.0%, Cr-18%, Ni-10%, Ti-0.6%, S-0.02%, P-0.035%, Fe-to 100%
Central tube: E110 Zr + 1% Nb alloy	Zr - 98.722%, Nb - 1.0%, Hf - 0.030%, Fe - 0.050%, Ni - 0.025%, Al - 0.008%, Ti - 0.007%, Si - 0.050%, C - 0.050%, N - 0.007%, O - 0.050%, H - 0.001÷0.002%
Guide tubes: Steel 08X18H10T	C - 0.08%, Si - 0.8%, Mn - 2.0%, Cr - 18%, Ni - 10%, Ti - 0.6%, S - 0.02%, P - 0.035%, Fe - to 100%
Control rods: B ₄ C	C- 20%, B ₁₁ - 64.08%, B ₁₀ - 15.92%

**Figure 15:** Color-set configuration for Kozloduy-6

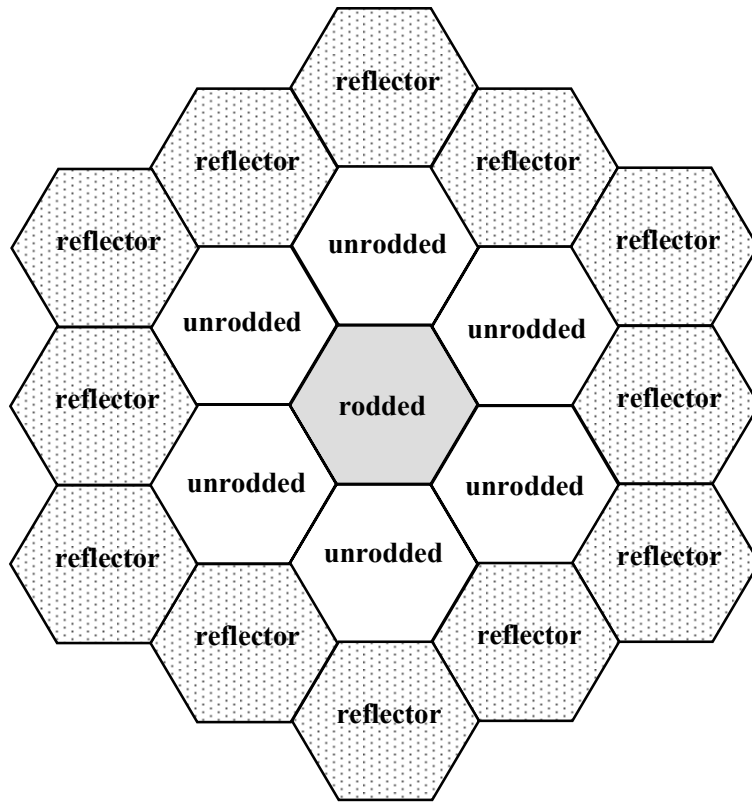
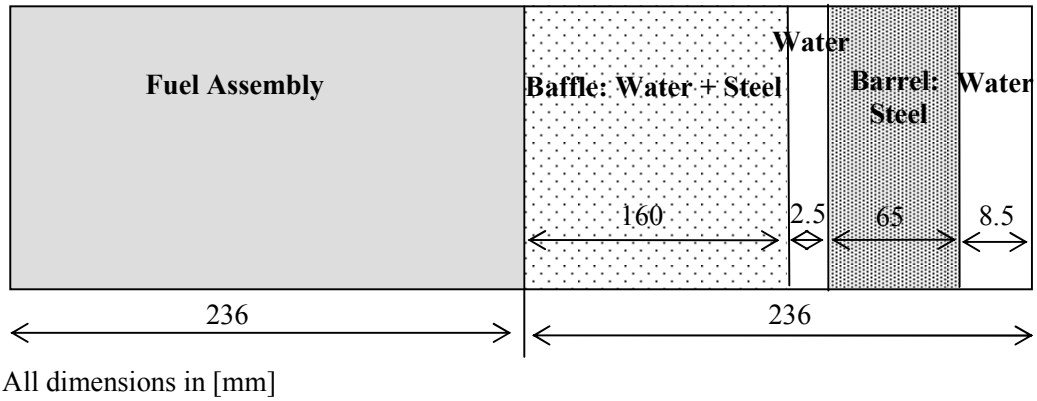


Figure 16: Color-set configuration for Kozloduy-6 (with reflector)



Material	Composition
Water (H ₂ O)	H - 11.19 % ; O - 88.81 %
Barrel: Steel 08X18H10T	C - 0.08%, Si - 0.8%, Mn - 2.0%, Cr - 18%, Ni - 10%, Ti - 0.6%, S - 0.02%, P - 0.035%, Fe - to 100%
Baffle	65.05% - Steel 08X18H10T 34.95% - H ₂ O

Figure 17: Kozloduy-6 radial reflector model – dimensions and material compositions

Chapter 4

DEFINITION OF EXERCISE I-3: CORE PHYSICS

This exercise consists of core calculations to propagate the defined below input uncertainties to output uncertainties in evaluated core parameters e.g. core reactivity, power distributions, and rod worth. The input uncertainties, which result in uncertainties in prediction of core parameters and which need to be accounted for and propagated, are arising from:

- Few-group lattice-average (homogenized) cross-section uncertainties;
- Approximations in the solution of the transport equation (basic modeling approximations);
- Numerical simplifications;
- Variations in geometry.

Understanding the uncertainties in key output reactor core parameters associated with steady state core simulation is important in regard to introducing appropriate design margins and deciding where efforts should be directed to reduce uncertainties [46]. The propagation of the input uncertainties through core calculations to determine uncertainties in output core parameters within the framework of Exercise I-3 requires utilization of a core simulator code. Participants can use/select their own core simulator codes in conjunction with their own UA and SA tools for the purposes of this exercise.

4.1 Discussion of input and target (output) uncertainties

In the current established calculation scheme for LWR design and safety analysis the lattice averaged (homogenized) few-group cross-sections are an input to core calculations. The few-group cross-section uncertainties (few-group covariance matrix) should be obtained by participants as output uncertainties within the framework of Exercise I-2. In Exercise I-3 the few-group cross-section uncertainties are input uncertainties and must be propagated to uncertainties in evaluated stand-alone neutronics core parameters. The propagation of the cross-section uncertainties is the most important part of Exercise I-3. If some participants want to take part only in Exercise I-3 (since they have already developed their core models for the benchmark problems discussed below) the benchmark team will provide “reference” input uncertainties (few-group cross sections supplemented with a few-group covariance matrix).

The other input uncertainties in Exercises I-3 are new uncertainties added during the core stand-alone calculations. The uncertainties due to the basic modeling simplifications include the currently accepted in the nuclear industry and regulation approximations for solving neutron balance equation. The established standard methodology for core calculation in routine LWR design and safety analysis is based on few-group (mostly two-group) diffusion method. Lately higher-order transport methods (such as S_n , P_n , SP_n , and MOC methods) and more energy groups are being applied to core analysis but they have not reached the maturity to be utilized in the industry and regulation as a routine design and safety analysis approach. The error due to use of diffusion approximation, and subsequently the uncertainty in core parameters due to use of diffusion approximation (diffusion vs. higher order transport approximation) can be assessed from the previous OECD/NEA benchmarks. Uncertainties are also introduced by the choice of the spatial discretization scheme utilized in the core simulator. The commonly used spatial discretization schemes are the different types of

nodal (finite-volume) methods, finite-difference methods, finite-element methods and etc. The participants are responsible of performing spatial discretization convergence studies with their core simulator codes in order to remove the uncertainties associated with numerical approximations (numerical method uncertainties) and reduce the uncertainties associated with the neutron transport method (physics uncertainties) used in core simulator codes.

There are also uncertainties associated with numerical simplifications in core modeling and variations in core geometry which need to be addressed and propagated. Information for these uncertainties for the different test models discussed below will be provided to the participants by the benchmark team.

4.2 Test problems

Three-dimensional (3-D) test problems are defined to be used within Exercise I-3, to assess the stand-alone neutronics core calculations and to determine the output core parameter uncertainties due to the input few-group lattice-averaged cross-section uncertainties, input geometry uncertainties, code modeling approximations uncertainties, and uncertainties due to numerical simplifications. The continuous energy Monte Carlo method is used for reference calculations assuming sufficient statistics, which guarantee k_{eff} and fission source convergence. The statistical uncertainties in the reference Monte Carlo calculations will be evaluated by the benchmark team. These example problems are developed and/or utilized on two different levels:

1. HZP core test cases defined for BWR PB-2 [6], PWR TMI-1 [7], and VVER-1000 [8] based on real plant core data. The boundary conditions are zero flux boundary conditions at radial and axial boundaries of the core models.

The information for the BWR core model is given in Figure 18 through Figure 24. The information for the PWR core model is given in Figure 25 through Figure 27. The information for the VVER core model is given in Figure 28 through Figure 30. These problems have to be analyzed at Hot Zero Power (HZP) conditions as defined in the Table 8.

For each problem the participants have to calculate the core multiplication factors (k_{eff}) and the relative pin powers (radial power and axial power distributions) as well as associated uncertainties due to core simulation within Exercise I-3.

2. Documented experimental benchmark plant cold critical data and critical lattice data.
 - a) BWR experimental plant cold critical data were reported in [50, 51]. The first reference will be provided in electronic format to the interested participants. This EPRI report provides reactor design and operating data for Cycle 1 and Cycle 2 of Quad Cities Unit 1 BWR. The attractive features of these data are that similar 7x7 BWR assembly designs to those utilized in the Cycle 1 of PB-2 are used for Cycle 1 of Quad Cities Unit 1. The benchmark cold critical data were taken during start-ups following outages, which were long enough to assume Xe-free conditions and they include core average exposure, reactor water temperature, rod pattern, and rising period. For the purposes of the OECD LWR UAM benchmark the cold critical state at the beginning of Cycle 1 (Exposure = 0.0 MWd/t) is used. The participants should calculate k_{eff} and associated uncertainties for this state.
 - b) PWR benchmark critical lattice data were reported in [52, 53]. At the beginning of 1970, a series of experiments with heterogeneous lattices of low-enriched UO_2 fuel rods was performed at B&W Research Center. For these experiments, the central region of the core closely resembled a 3x3

array of PWR fuel assemblies with fuel rods arranged in a 15x15 lattice (similar to TMI-1 core). Loading 2 is selected for the purposes of the OECD LWR UAM benchmark. The necessary data for modeling can be obtained from [52] (NEA/NSC/DOC(95)03/IV – LEU-COMP-THERM-008). The participants should calculate k_{eff} of the core and relative rod-by-rod power densities (fission rate distributions) of the central assembly (using pin power reconstruction methods available in their core simulator codes) as well as the associated uncertainties in these parameters.

- c) VVER-1000 benchmark critical lattice data were reported in [52]. Ten experiments were performed in 1998 on the experimental zero-power reactor LR-0 (Nuclear Research Institute Řež plc, Czech Republic). The core was assembled from 6 VVER-1000 fuel assemblies and the experiments were carried out at atmospheric pressure and “room” temperature. Case 3 is selected for the purposes of the OECD LWR UAM benchmark. The necessary data for modeling can be obtained from [52] (NEA/NSC/DOC(95)03/IV – LEU-COMP-THERM-086). The participants should calculate k_{eff} of the core and the associated uncertainties.

In summary this exercise is focused on stand-alone neutronics core calculations and associated prediction uncertainties. It does not analyze uncertainties related to cycle and depletion calculations. No feedback modeling is assumed, thus it will address the propagation of uncertainties associated with few-group cross-section generation but not cross-section modeling i.e. methodologies used for cross-section parameterization as a function of history and instantaneous variables.

Exercise I-3 propagates the input uncertainty obtained from Exercise I-2 (few-group cross-section covariance matrix), and in addition introduces new input uncertainties (geometry variations, numerical simplifications, and modeling approximations) to obtain prediction uncertainties in stand-alone core neutronics parameters.

The output uncertainty of Exercise I-3 is propagated in Exercises II-1, II-2, II-3, and III-1 and III-3.

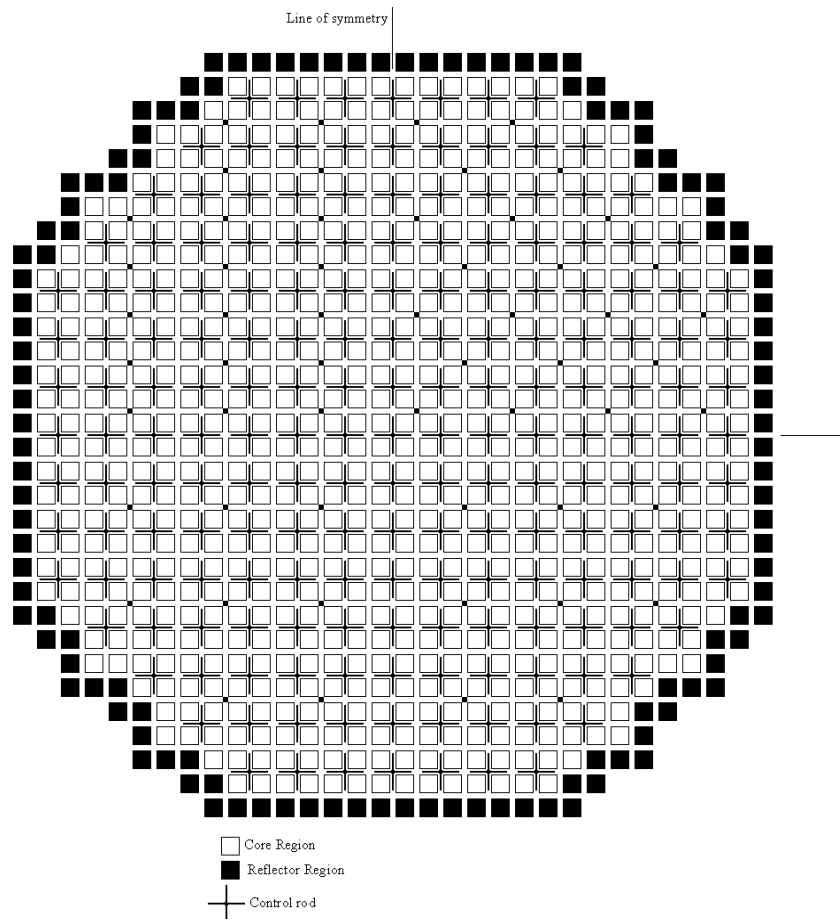


Figure 18: PB-2 reactor core cross-sectional view

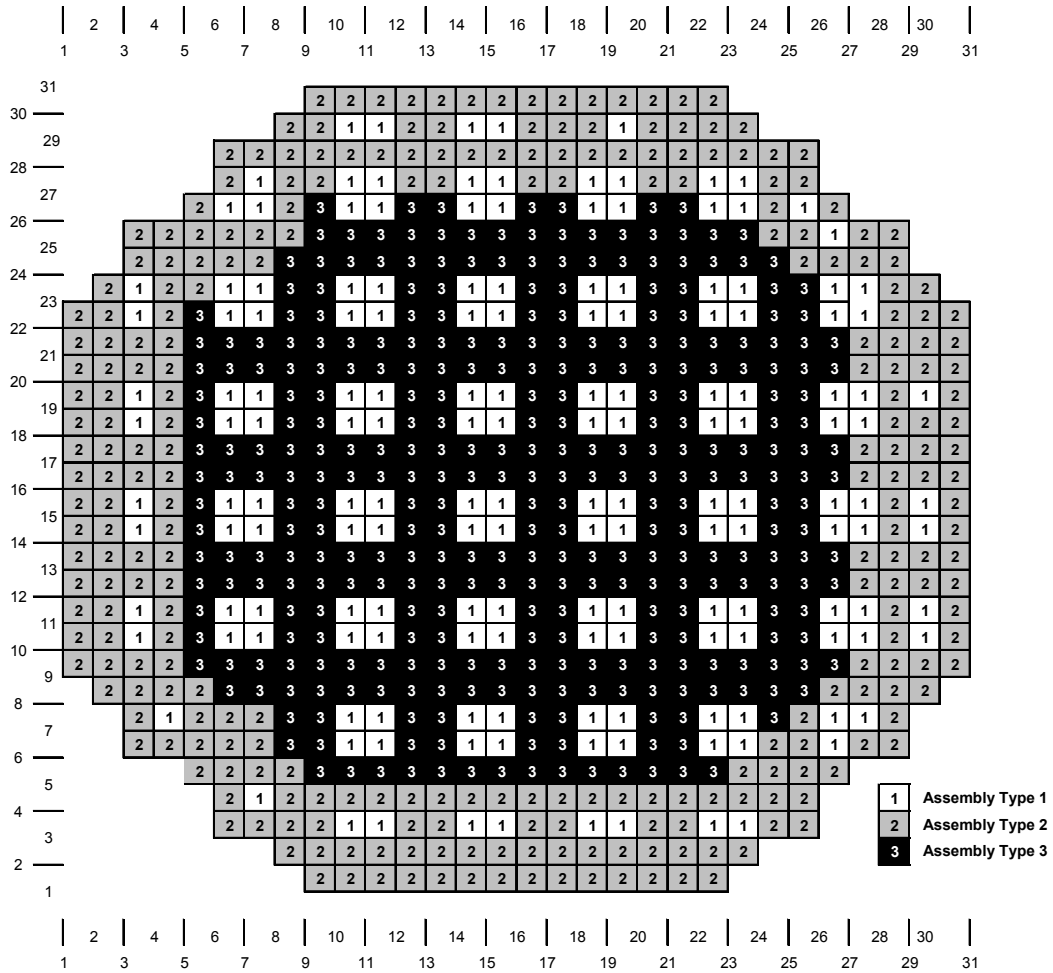


Figure 19: PB-2 initial core loading

Rod type	Number of rods	Pellet density		Stack density (g/cm ³)	Gd ₂ O ₃ (g)	UO ₂ (g)	Stack length (cm)
		UO ₂ (g/cm ³)	UO ₂ +Gd ₂ O ₃ (g/cm ³)				
1	31	10.42	-	10.34	0	4548	365.76
2	17	10.42	-	10.34	0	4548	365.76
2s	01	10.42	-	10.34	0	4140	330.2

Pellet outer diameter = 1.23698 cm.

Cladding = Zircaloy-2, 1.43002 cm outer diameter × .08128 cm wall thickness, all rods.

Gas plenum length = 40.64 cm.

Assembly design for Type 1 initial fuel

Rod type	²³ U (wt.%)	Gd ₂ O ₃ (wt.%)	No. of rods
1	1.33	0	31
2	0.71	0	18

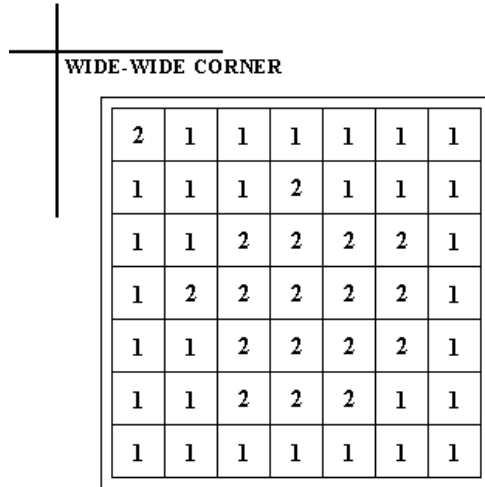


Figure 20: PB-2 assembly design - Type 1 initial fuel

Rod type	Number of rods	Pellet density		Stack density (g/cm ³)	Gd ₂ O ₃ (g)	UO ₂ (g)	Stack length (cm)
		UO ₂ (g/cm ³)	UO ₂ +Gd ₂ O ₃ (g/cm ³)				
1	26	10.42	—	10.32	0	4 352	365.76
2	11	10.42	—	10.32	0	4 352	365.76
3	6	10.42	—	10.32	0	4 352	365.76
4	1	10.42	—	10.32	0	4 352	365.76
5A	2	—	10.29	10.19	129	4 171	365.76
6C	1	—	10.29	10.19	117	3 771	330.20
7E	1	10.42	10.25	10.28	43	4 292	365.76
8D	1	10.42	10.25	10.19	129	4 172	365.76

Pellet outer diameter = 1.21158 cm.

Cladding = Zircaloy-2, 1.43002 cm outer diameter × .09398 cm wall thickness, all rods.

Gas plenum length = 40.132 cm.

Assembly design for Type 3 initial fuel

Rod type	²³⁵ U (wt.%)	Gd ₂ O ₃ (wt.%)	No. of rods
1	2.93	0	26
2	1.94	0	11
3	1.69	0	6
4	1.33	0	1
5A	2.93	3.0	2
6C	2.93	3.0	1
7E	2.93	4.0	1
8D	1.94	4.0	1

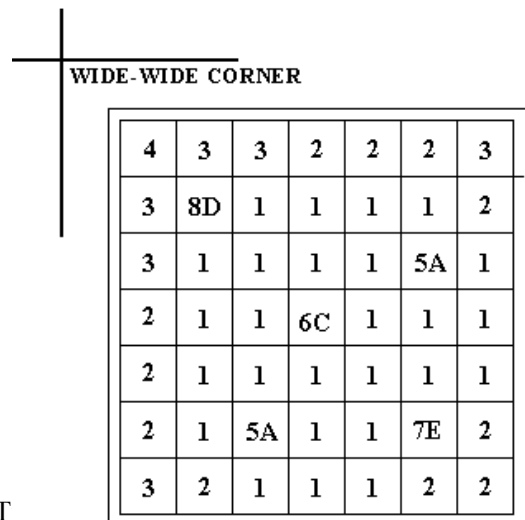


Figure 21: PB-2 assembly design - T

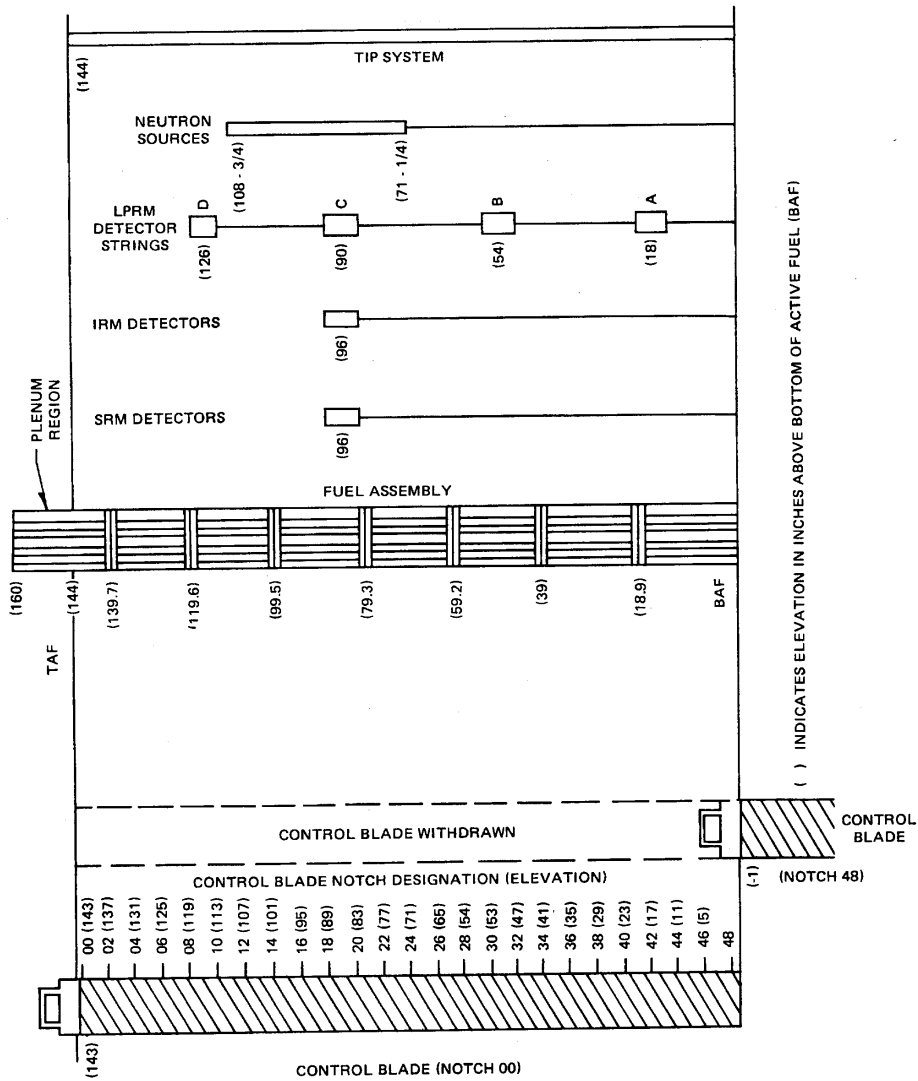


Figure 23: Elevation of core components for PB-2

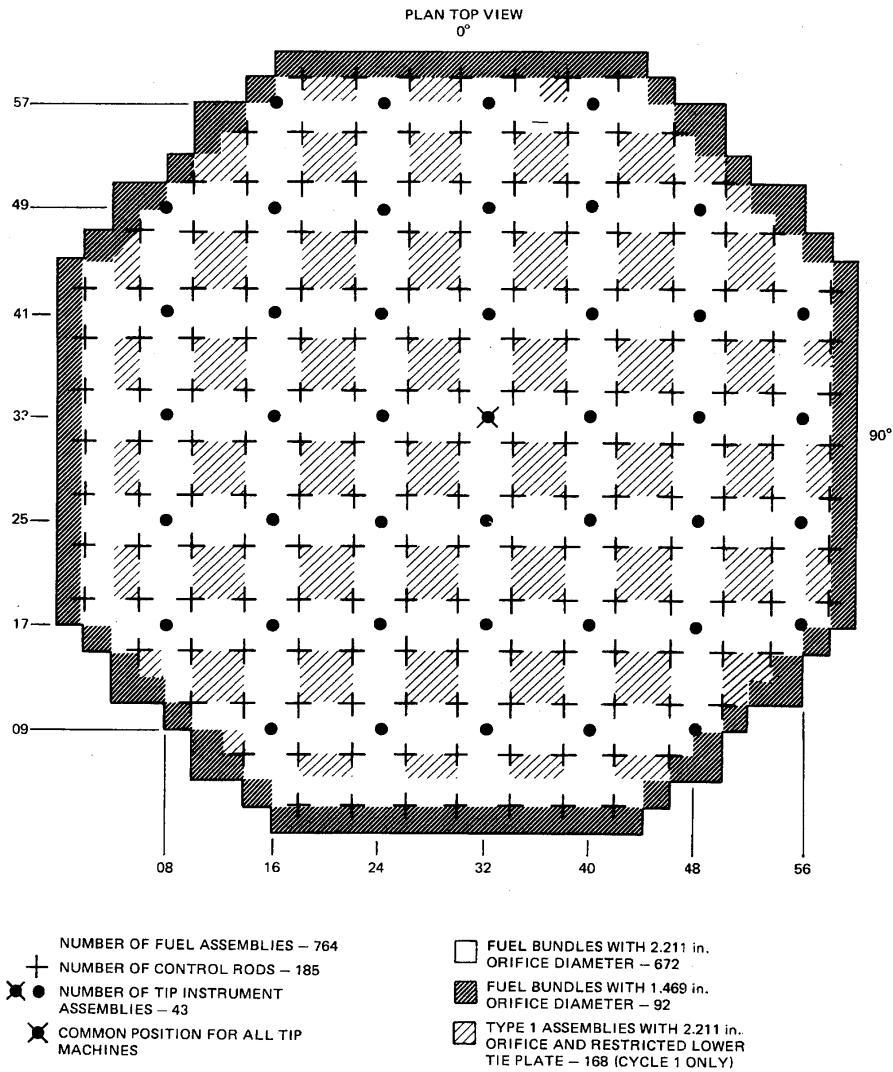
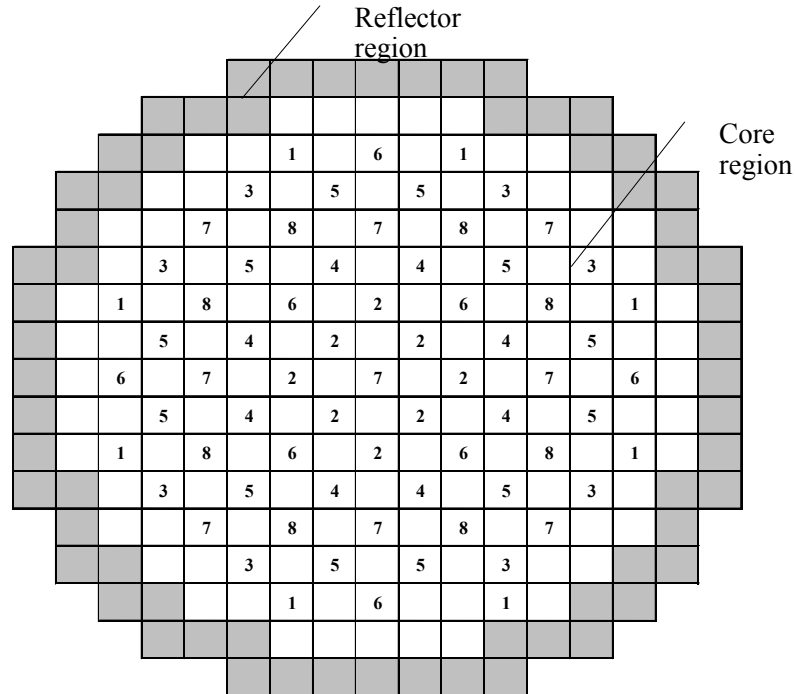
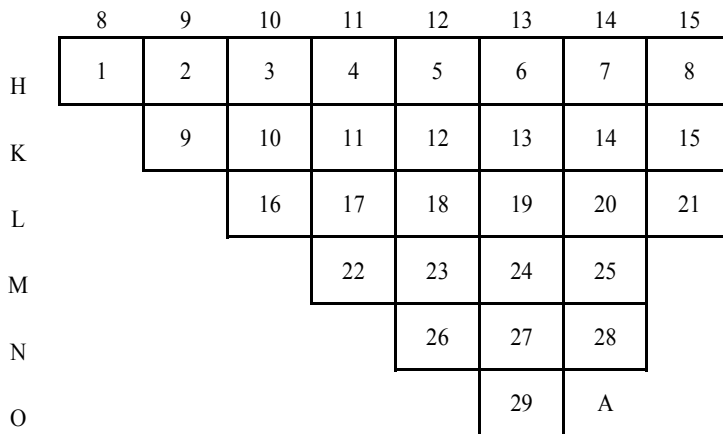


Figure 24: PB-2 - core orificing and TIP system arrangement



Parameter	Value	Bank	No. rods	Purpose
Total number of fuel assemblies	177	1	8	Safety
Total number of reflector assemblies	64	2	8	Safety
Fuel assembly pitch, mm	218.110	3	8	Safety
Gap between fuel assemblies, mm	1.702	4	8	Safety
Active core length, mm	3571.20	5	12	Regulating
Total core length, mm	4007.42	6	8	Regulating
		7	9	Regulating
		8	8	APSR

Figure 25: TMI-1 reactor core cross-sectional view and characteristics



A -Type of fuel assembly

Assembly	Characteristics		
1	4.00 w/o	No BP	No Gd pins
2	4.95 w/o	3.5 % BP	4 Gd pins
3	5.00 w/o	3.5 % BP	4 Gd pins
4	4.95 w/o	3.5 % BP	4 Gd pins
5	4.40 w/o	No BP	No Gd pins
6	5.00 w/o	3.5 % BP	4 Gd pins
7	4.85 w/o	No BP	4 Gd pins
8	4.85 w/o	No BP	4 Gd pins
9	4.95 w/o	3.5 % BP	4 Gd pins
10	4.95 w/o	3.5 % BP	4 Gd pins
11	4.85 w/o	3.5 % BP	4 Gd pins
12	4.95 w/o	3.5 % BP	4 Gd pins
13	5.00 w/o	3.5 % BP	4 Gd pins
14	5.00 w/o	No BP	8 Gd pins
15	4.95 w/o	No BP	8 Gd pins
16	4.95 w/o	3.5 % BP	4 Gd pins
17	4.95 w/o	3.5 % BP	4 Gd pins
18	4.95 w/o	3.5 % BP	4 Gd pins
19	5.00 w/o	3.5 % BP	4 Gd pins
20	4.40 w/o	No BP	No Gd pins
21	4.85 w/o	3.5 % BP	4 Gd pins
22	4.40 w/o	No BP	No Gd pins
23	4.95 w/o	3.5 % BP	No Gd pins
24	4.95 w/o	3.5 % BP	4 Gd pins
25	5.00 w/o	No BP	8 Gd pins
26	5.00 w/o	No BP	4 Gd pins
27	5.00 w/o	No BP	No Gd pins
28	4.95 w/o	3.5 % BP	4 Gd pins
29	5.00 w/o	No BP	4 Gd pins

Figure 26: TMI-1 – definition of fuel assembly types

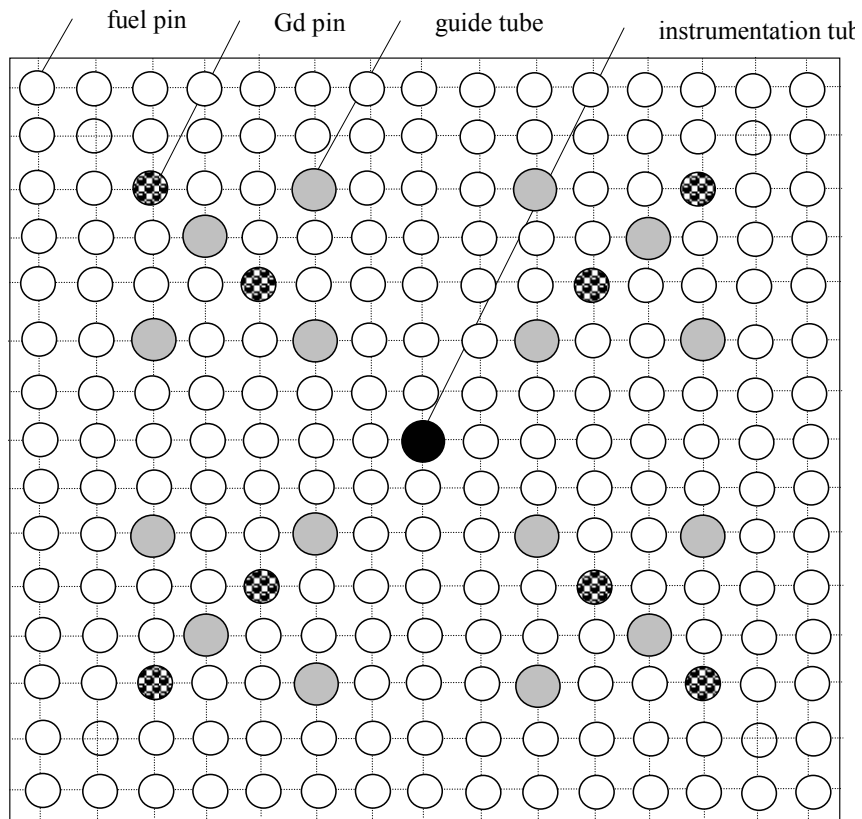
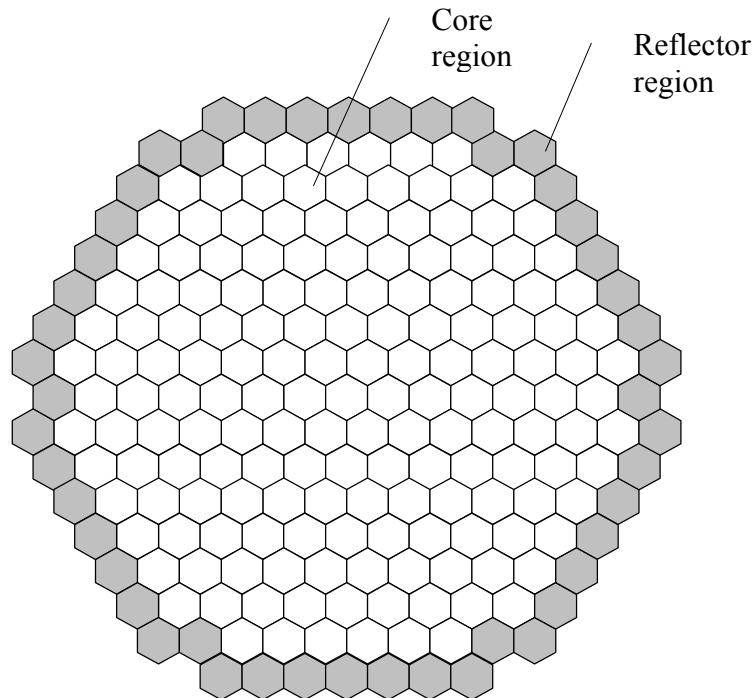
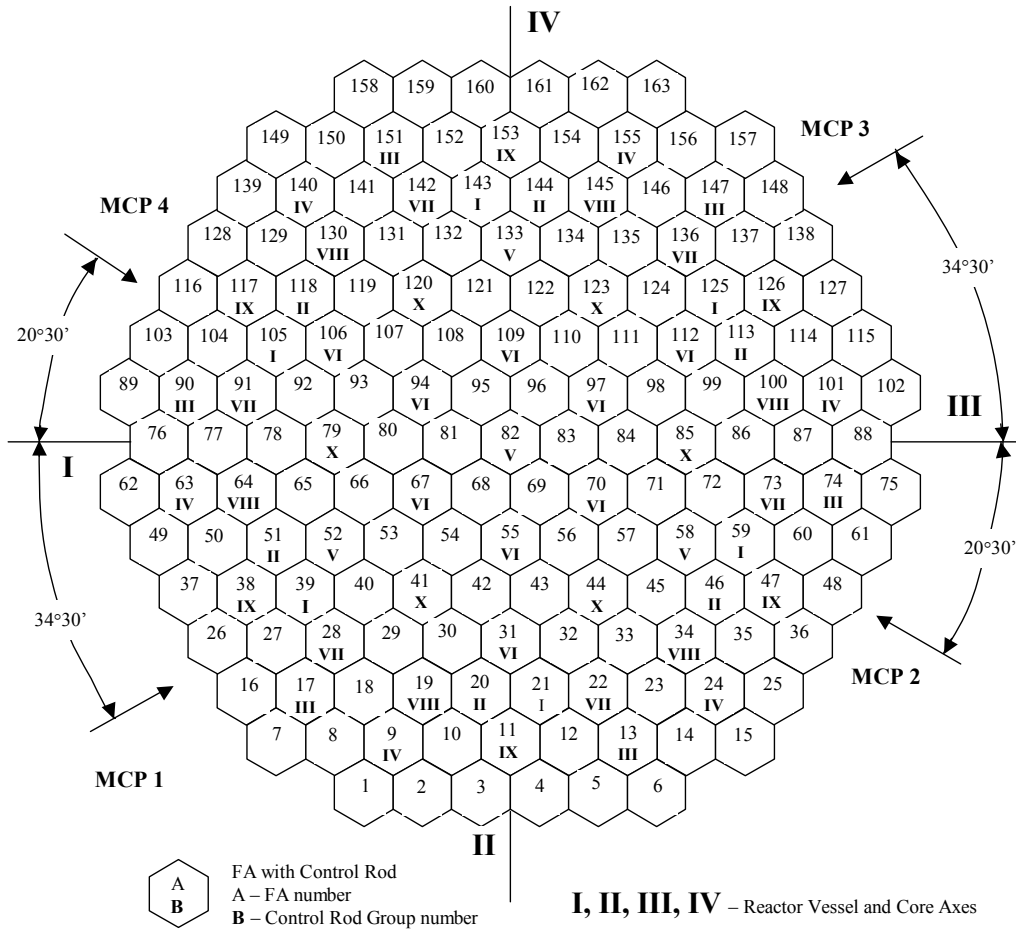


Figure 27: TMI-1 assembly design with 8 Gd pins



Parameter	Value
Total number of fuel assemblies	163
Total number of reflector assemblies	48
FA wrench size, mm	234
FA lattice pitch, mm	236
Fuel rod total length, mm	3837
Fuel rod active length (cold state), mm	3530
Fuel rod active length (hot state), mm	3550

Figure 28: Kozloduy-6 reactor core cross-sectional view and characteristics



Bank	No. of rods	Purpose
I	6	Safety
II	6	Safety
III	6	Safety
IV	6	Safety
V	4	Part-length
VI	9	Safety
VII	6	Safety
VIII	6	Safety
IX	6	Safety
X	6	Regulating

Figure 29: Kozloduy-6 – control rod arrangement

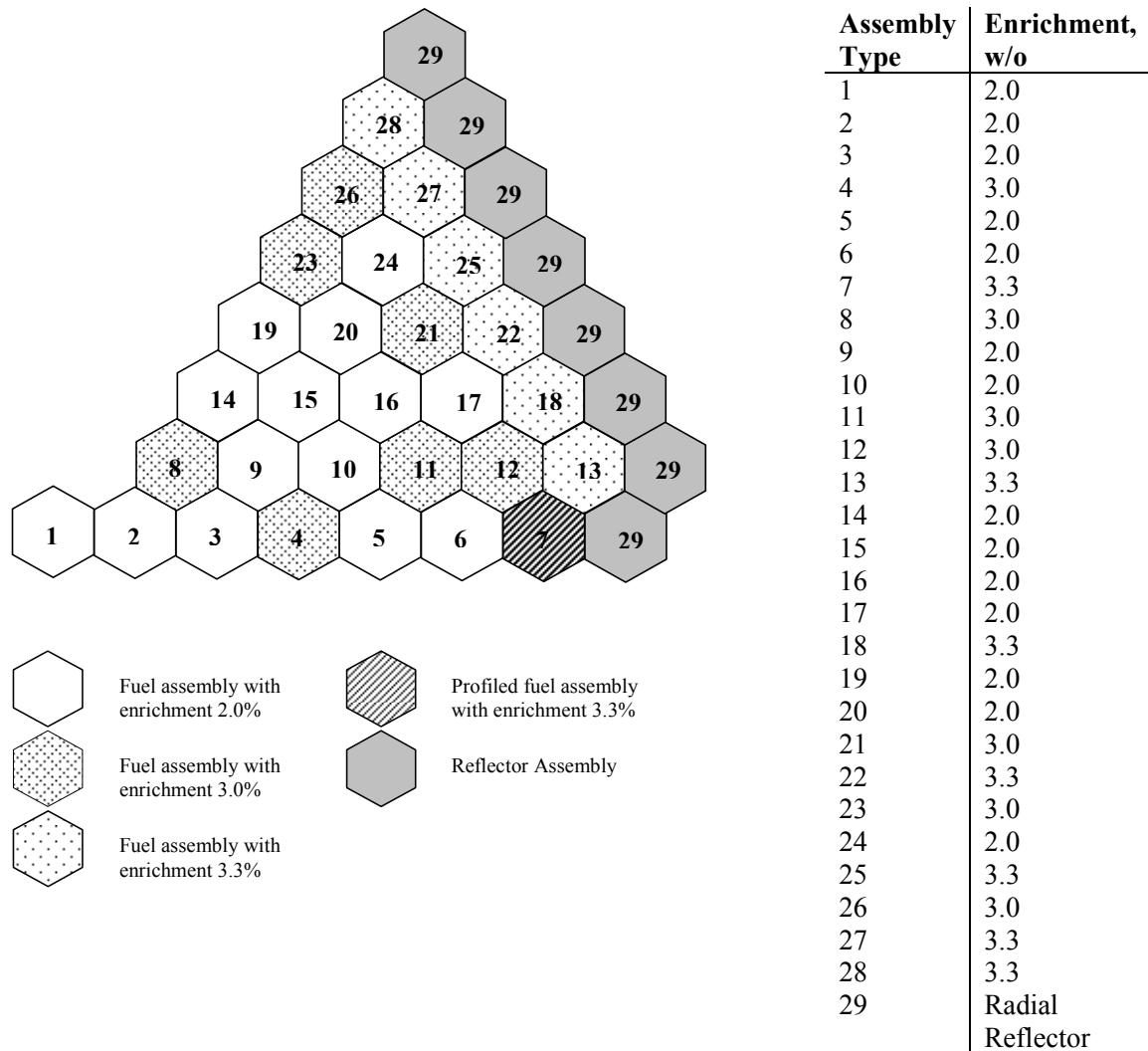


Figure 30: Kozloduy-6 – core loading

Chapter 5

REQUESTED OUTPUT

5.1 Introduction

The results of Phase I analysis will be presented in a benchmark analysis report, which will be made available in both a hard copy and an electronic form.

Participants should provide the output information with the given requirements:

- Results should be submitted in an electronic format according to templates, which will be provided to participants by the benchmark team.
- All data should be in SI units.

5.2 Results for Exercise I-1

The following results will be compared for Exercise I-1:

Set 1: Two-dimensional fuel pin-cell test problems representatives of PB-2 BWR, TMI-1 PWR, and Kozloduy-6 VVER-1000

- One group effective cross-section uncertainties for the present nuclides as defined by Eq.3 in Section 2.4 (these total effective relative errors corresponding to the typical neutron flux spectrum in a LWR pin cell are used to characterize the multigroup covariance matrices);
- K_{inf} and associated uncertainties¹¹;
- Absorption reaction rates for ^{234}U , ^{235}U , and ^{238}U and associated uncertainties;
- Fission reaction rates for ^{234}U , ^{235}U , and ^{238}U and associated uncertainties.

Set 2: Fuel pin-cell test problems from the KRITZ-2 LEU critical experiments

- K_{inf} ;
- Absorption reaction rates for ^{234}U , ^{235}U , and ^{238}U and associated uncertainties;
- Fission reaction rates for ^{234}U , ^{235}U , and ^{238}U and associated uncertainties.

Set 3: Core test problems from the KRITZ-2 LEU critical experiments

- K_{eff} and associated uncertainties at “room” temperature;
- K_{eff} and associated uncertainties at “elevated” temperature;
- Relative rod powers for the rods and associated uncertainties.

Set 4: VVER-1000 assembly lattice test problems from the RRC KI VVER physics experiments

- K_{eff} and associated uncertainties at “room” temperature;
- Relative radial fission reaction rate distribution and associated uncertainties for the Case 9

¹¹ Associated uncertainties are in term of standard deviation.

5.3 Results for Exercise I-2

The following results will be compared for Exercise I-2:

Set 1: 2-D assembly model with reflective boundary conditions

- One group effective uncertainties;
- The output uncertainties of the following few group assembly homogenized parameters will be compared:
 - a) Macroscopic cross-sections of different reactions;
 - b) ADFs, CDFs, Form Functions;
 - c) Kinetics and delayed neutron parameters;
- K_{inf} and associated uncertainties;
- Absorption reaction rates and associated uncertainties;
- Fission reaction rates and associated uncertainties;

Set 2: 1-D assembly/reflector model

- The output uncertainties of the following few group reflector homogenized parameters will be compared:
 - a) Macroscopic cross-sections of different reactions;
 - b) ADFs.

Set 3: 2-D assembly color sets (mini-cores)

- Mini-core multiplication factors (K_{eff}) and associated uncertainties;
- Mini-core relative pin powers and associated uncertainties.

5.4 Results for Exercise I-3

The following results will be compared for Exercise I-3:

- K_{eff} and associated uncertainties;
- Core axial power distribution and associated uncertainties;
- Radial power distribution and associated uncertainties.

Output sample

PB-2 BWR Results

A PEACH BOTTOM - 2 BWR RESULTS FROM CODE "XXXXXXXX", EXERCISE I-3

B STEADY STATE RESULTS

B.1 $K_{eff} = 1.00000$

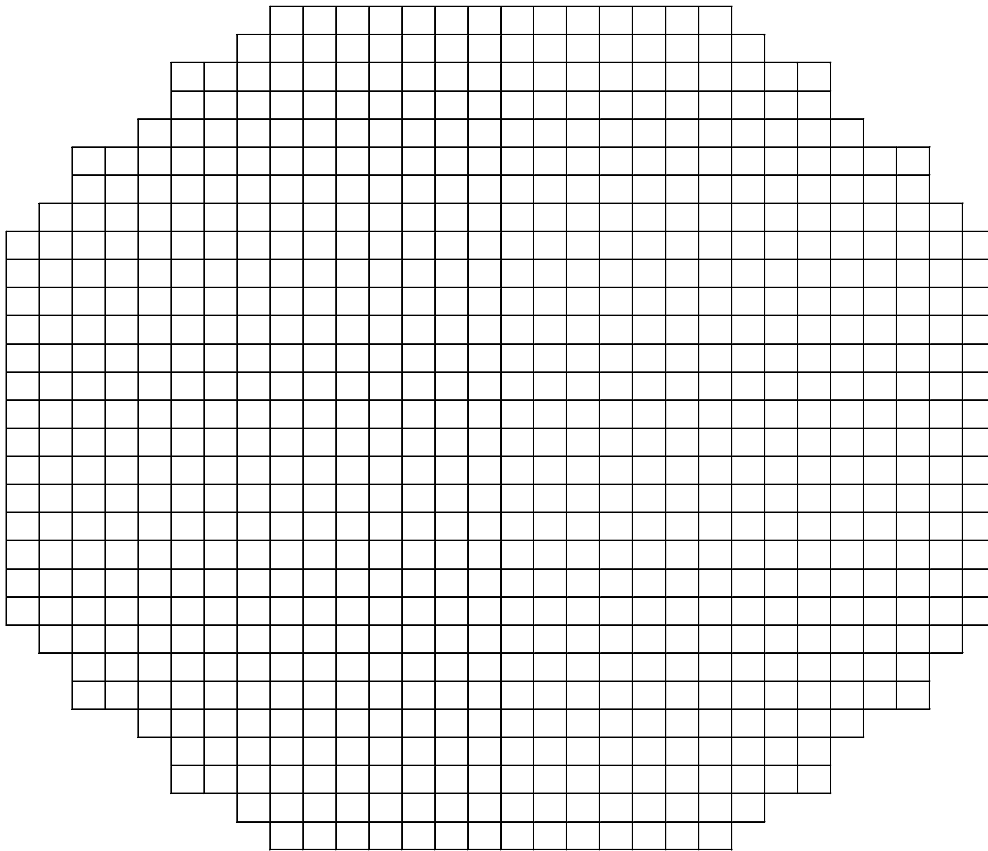


Figure 31: Form for radial power distribution for PB-2 BWR results

Bottom

1	2	3	4	5	6	7	8	9	10	11	12
13	14	15	16	17	18	19	20	21	22	23	24

Top

Figure 32: Form for axial power distribution for PB-2 BWR results

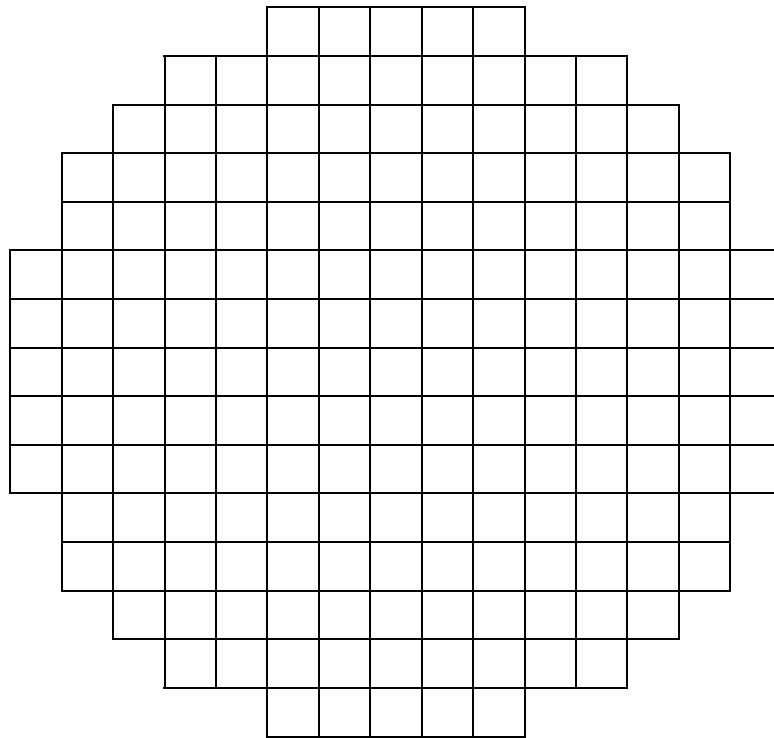
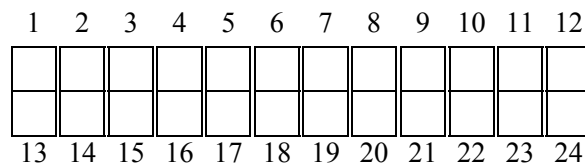


Figure 33: Form for radial power distribution for TMI-1 PWR results

Bottom



Top

Figure 34: Form for axial power distribution for TMI-1 PWR results

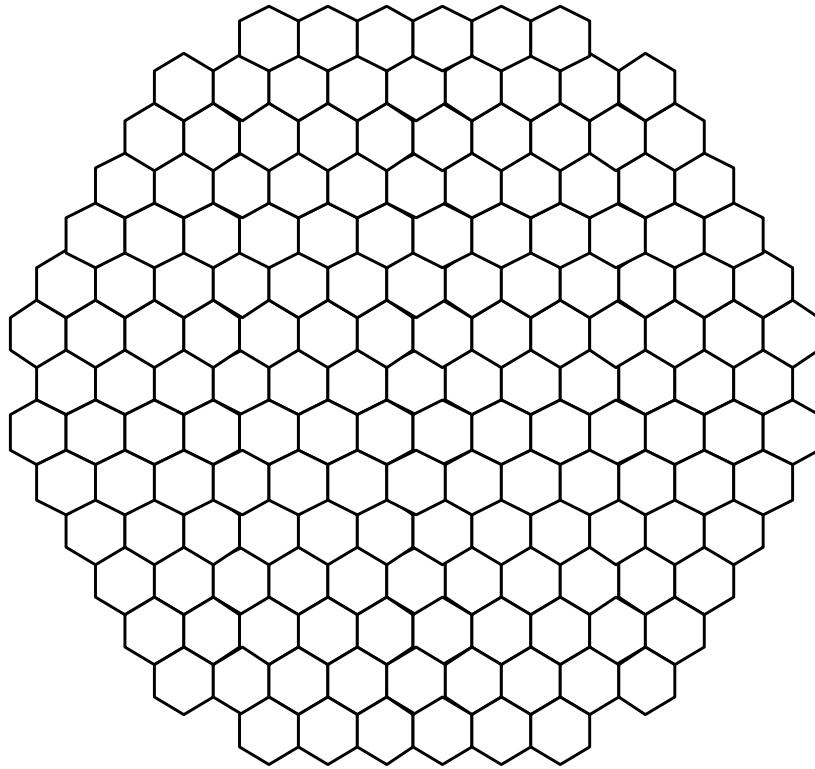


Figure 35: Form for radial power distribution for Kozloduy-6 results



Figure 36: Form for axial power distribution for Kozloduy-6 results

Chapter 6

CONCLUSIONS

The objective of the OECD LWR UAM activity is to establish an internationally accepted benchmark framework to compare, assess and further develop different uncertainty analysis methods associated with the design, operation and safety of LWRs. As a result the LWR UAM benchmark will help to address current nuclear power generation industry and regulation needs and issues related to practical implementation of risk informed regulation. The realistic evaluation of consequences must be made with best estimate coupled codes, but to be meaningful, such results should be supplemented by an uncertainty analysis. The use of coupled codes allows to avoid unnecessary penalties due to incoherent approximations in the traditional decoupled calculations, and to obtain more accurate evaluation of margins regarding licensing limit. This becomes important for licensing power upgrades, improved fuel assembly and control rod designs, higher burn-up and others issues related to operating LWRs as well as to the new Generation 3+ designs being licensed now (ESBWR, AP-1000, EPR-1600 and etc.). Establishing such internationally accepted LWR UAM benchmark framework offers the possibility to accelerate the licensing process when using best estimate methods.

The proposed technical approach is to establish a benchmark for uncertainty analysis in best-estimate modeling and coupled multi-physics and multi-scale LWR analysis, using as bases a series of well defined problems with complete sets of input specifications and reference experimental data. The objective is to determine the uncertainty in LWR system calculations at all stages of coupled reactor physics/thermal hydraulics calculation. The full chain of uncertainty propagation from basic data, engineering uncertainties, across different scales (multi-scale), and physics phenomena (multi-physics) will be tested on a number of benchmark exercises for which experimental data is available and for which the power plant details have been released.

This report presents benchmark specifications for Phase I (Neutronics Phase) of the OECD LWR UAM benchmark in a format similar to the previous OECD/NRC benchmark specifications. The Phase I consists of the following exercises:

Exercise 1 (I-1): “Cell Physics” focused on the derivation of the multi-group microscopic cross-section libraries

Exercise 2 (I-2): “Lattice Physics” focused on the derivation of the few-group macroscopic cross-section libraries

Exercise 3 (I-3): “Core Physics” focused on the core steady state stand-alone neutronics calculations

These exercises follow those established in the industry and regulation routine calculation scheme for LWR design and safety analysis. This phase is focused on understanding uncertainties in the prediction of key reactor core parameters associated with LWR stand-alone neutronics core simulation. Such uncertainties occur due to input data uncertainties, modeling errors, and numerical approximations. Understanding the uncertainties in key output reactor core parameters associated with steady state core simulation is important with regard to introducing appropriate design margins and deciding where efforts should be directed to reduce uncertainties. The obtained output uncertainties from Phase I of the OECD LWR UAM benchmark will be utilized as input uncertainties in the remaining two phases – Phase II (Core Phase) and Phase III (System Phase).

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Appendix I

List of nuclides with covariance information in 44GROUPV5COV set

Nuclide	Data source	Nuclide	Data source
²⁷ Al	ENDF/B-V	⁵⁵ Mn	ENDF/B-V
²⁴¹ Am	ENDF/B-V	¹⁴ N	ENDF/B-V
¹⁹⁷ Au	ENDF/B-V	²³ Na	ENDF/B-V
¹⁰ B	ENDF/B-V	Ni	ENDF/B-V
C	ENDF/B-V	²³⁷ Np	ENDF/B-V
C-graphite	ENDF/B-V	¹⁶ O	ENDF/B-V
²⁵² Cf	χ only	Pb	ENDF/B-V
⁵⁹ Co	ENDF/B-V	²³⁹ Pu	ENDF/B-V
Cr	ENDF/B-V	²⁴⁰ Pu	ENDF/B-V
¹⁹ F	ENDF/B-V	²⁴¹ Pu	ENDF/B-V
Fe	ENDF/B-V	²⁴² Pu	ENDF/B-V
¹ H	ENDF/B-V	Si	ENDF/B-V
H-ZrH	ENDF/B-V	²³² Th	ENDF/B-V
H-poly	ENDF/B-V	²³³ U	χ only
¹¹⁵ In	ENDF/B-V	²³⁵ U	ENDF/B-V
⁶ Li	ENDF/B-V	²³⁸ U	ENDF/B-V
⁷ Li	ENDF/B-V		

Appendix II

List of nuclides with covariance information in 44GROUPV6COV set

Nuclide	Data source	Nuclide	Data source
²⁷ Al	ENDF/B-VI	⁷ Li	ENDF/B-VI
²⁴¹ Am	ENDF/B-VI	⁵⁵ Mn	ENDF/B-VI
¹⁹⁷ Au	ENDF/B-VI	²³ Na	ENDF/B-VI
¹⁰ B	ENDF/B-V	⁹³ Nb	ENDF/B-VI
¹¹ B	JENDL 3.3	⁵⁸ Ni	ENDF/B-VI
²⁰⁹ Bi	ENDF/B-VI	⁶⁰ Ni	ENDF/B-VI
C	ENDF/B-VI	⁶¹ Ni	ENDF/B-VI
C-graphite	ENDF/B-VI	⁶² Ni	ENDF/B-VI
²⁵² Cf	χ only	⁶⁴ Ni	ENDF/B-VI
⁵⁹ Co	ENDF/B-VI	¹⁶ O	JENDL 3.3
⁵⁰ Cr	ENDF/B-VI	²⁰⁶ Pb	ENDF/B-VI
⁵² Cr	ENDF/B-VI	²⁰⁷ Pb	ENDF/B-VI
⁵³ Cr	ENDF/B-VI	²⁰⁸ Pb	ENDF/B-VI
⁵⁴ Cr	ENDF/B-VI	²³⁹ Pu	ENDF/B-V
⁶³ Cu	ENDF/B-VI	²⁴⁰ Pu	JENDL 3.3
⁶⁵ Cu	ENDF/B-VI	²⁴¹ Pu	JENDL 3.3
¹⁹ F	ENDF/B-VI	²⁴² Pu	ENDF/B-VI
⁵⁴ Fe	ENDF/B-VI	¹⁸⁵ Re	ENDF/B-VI
⁵⁶ Fe	ENDF/B-VI	¹⁸⁷ Re	ENDF/B-VI
⁵⁷ Fe	ENDF/B-VI	⁴⁵ Sc	ENDF/B-VI
⁵⁸ Fe	ENDF/B-VI	Si	ENDF/B-VI
¹ H	JENDL 3.3	²⁸ Si	ENDF/B-VI
H-ZrH	JENDL 3.3	²⁹ Si	ENDF/B-VI
H-poly	JENDL 3.3	³⁰ Si	ENDF/B-VI
Hfreegas	JENDL 3.3	²³² Th	ENDF/B-VII Beta 2
² H	CENDL 2	²³³ U	ENDF/B-VII Beta 2
Dfreegas	CENDL 2	²³⁵ U	JENDL 3.3
³ H	JEF 3.1	²³⁸ U	JENDL 3.3
³ He	CENDL 2	V	ENDF/B-VI
In	ENDF/B-VI	⁸⁹ Y	ENDF/B-VI

Appendix III

List of nuclides with covariance information in 44GROUPV5REC set

Nuclide	Data source	Nuclide	Data source	Nuclide	Data source
¹⁰⁷ Ag	Mughabghab	²⁴⁷ Cm	Mughabghab	¹²⁹ I	Mughabghab
¹⁰⁹ Ag	Mughabghab	²⁴⁸ Cm	Mughabghab	¹³⁰ I	Mughabghab
¹¹¹ Ag	Mughabghab	⁵⁹ Co	ENDF/B-V	¹³¹ I	Mughabghab
²⁷ Al	ENDF/B-V	Cr	ENDF/B-V	¹¹⁵ In	ENDF/B-V
²⁴¹ Am	ENDF/B-VI	¹³³ Cs	Mughabghab	K	Mughabghab
²⁴² Am	Mughabghab	¹³⁴ Cs	Mughabghab	⁷⁸ Kr	Mughabghab
^{242m} Am	Mughabghab	¹³⁵ Cs	Mughabghab	⁸⁰ Kr	Mughabghab
²⁴³ Am	Mughabghab	¹³⁷ Cs	Mughabghab	⁸² Kr	Mughabghab
⁷⁵ As	Mughabghab	Cu	ENDF/B-VI	⁸³ Kr	Mughabghab
¹⁹⁷ Au	ENDF/B-V	¹⁶⁰ Dy	Mughabghab	⁸⁴ Kr	Mughabghab
¹⁰ B	ENDF/B-V	¹⁶¹ Dy	Mughabghab	⁸⁵ Kr	Mughabghab
¹¹ B	JENDL 3.3	¹⁶² Dy	Mughabghab	⁸⁶ Kr	Mughabghab
¹³⁴ Ba	Mughabghab	¹⁶³ Dy	Mughabghab	¹³⁹ La	Mughabghab
¹³⁵ Ba	Mughabghab	¹⁶⁴ Dy	Mughabghab	¹⁴⁰ La	Mughabghab
¹³⁶ Ba	Mughabghab	¹⁶⁶ Er	Mughabghab	⁶ Li	ENDF/B-V
¹³⁷ Ba	Mughabghab	¹⁶⁷ Er	Mughabghab	⁷ Li	ENDF/B-V
¹³⁸ Ba	Mughabghab	²⁵³ Es	Mughabghab	¹⁷⁵ Lu	Mughabghab
¹⁴⁰ Ba	Mughabghab	¹⁵¹ Eu	Mughabghab	¹⁷⁶ Lu	Mughabghab
⁹ Be	Mughabghab	¹⁵² Eu	Mughabghab	Mg	Mughabghab
Be-bound	Mughabghab	¹⁵³ Eu	Mughabghab	⁵⁵ Mn	ENDF/B-VI
²⁰⁹ Bi	ENDF/B-VI	¹⁵⁴ Eu	Mughabghab	Mo	Mughabghab
²⁴⁹ Bk	Mughabghab	¹⁵⁵ Eu	Mughabghab	⁹⁴ Mo	Mughabghab
⁷⁹ Br	Mughabghab	¹⁹ F	ENDF/B-V	⁹⁵ Mo	Mughabghab
⁸¹ Br	Mughabghab	Fe	ENDF/B-V	⁹⁶ Mo	Mughabghab
C	ENDF/B-V	Ga	Mughabghab	⁹⁷ Mo	Mughabghab
C-graphite	ENDF/B-V	¹⁵² Gd	ENDF/B-VII Beta 2	¹⁴ N	ENDF/B-V
Ca	Mughabghab	¹⁵⁴ Gd	ENDF/B-VII Beta 2	¹⁵ N	Mughabghab
Cd	Mughabghab	¹⁵⁵ Gd	ENDF/B-VII Beta 2	²³ Na	ENDF/B-V
¹⁰⁶ Cd	Mughabghab	¹⁵⁶ Gd	ENDF/B-VII Beta 2	⁹³ Nb	ENDF/B-V
¹⁰⁸ Cd	Mughabghab	¹⁵⁷ Gd	ENDF/B-VII Beta 2	⁹⁴ Nb	Mughabghab
¹¹⁰ Cd	Mughabghab	¹⁵⁸ Gd	ENDF/B-VII Beta 2	⁹⁵ Nb	Mughabghab
¹¹¹ Cd	Mughabghab	¹⁶⁰ Gd	ENDF/B-VII Beta 2	¹⁴² Nd	Mughabghab
¹¹² Cd	Mughabghab	⁷² Ge	Mughabghab	¹⁴³ Nd	Mughabghab
¹¹³ Cd	Mughabghab	⁷³ Ge	Mughabghab	¹⁴⁴ Nd	Mughabghab
¹¹⁴ Cd	Mughabghab	⁷⁴ Ge	Mughabghab	¹⁴⁵ Nd	Mughabghab
¹¹⁶ Cd	Mughabghab	⁷⁶ Ge	Mughabghab	¹⁴⁶ Nd	Mughabghab
¹⁴⁰ Ce	Mughabghab	¹ H	ENDF/B-V	¹⁴⁷ Nd	Mughabghab
¹⁴¹ Ce	Mughabghab	H-ZrH	ENDF/B-V	¹⁴⁸ Nd	Mughabghab
¹⁴² Ce	Mughabghab	H-poly	ENDF/B-V	¹⁵⁰ Nd	Mughabghab
¹⁴³ Ce	Mughabghab	² H	CENDL 2	Ni	ENDF/B-V
¹⁴⁴ Ce	Mughabghab	³ H	JEF 3.1	²³⁷ Np	ENDF/B-V
²⁴⁹ Cf	Mughabghab	³ He	CENDL 2	¹⁶ O	ENDF/B-V
²⁵⁰ Cf	Mughabghab	⁴ He	Mughabghab	¹⁷ O	Mughabghab
²⁵¹ Cf	Mughabghab	Hf	Mughabghab	³¹ P	Mughabghab
²⁵² Cf	Mughabghab	¹⁷⁴ Hf	Mughabghab	²³¹ Pa	Mughabghab
²⁵³ Cf	Mughabghab	¹⁷⁶ Hf	Mughabghab	²³³ Pa	Mughabghab
Cl	Mughabghab	¹⁷⁷ Hf	Mughabghab	Pb	ENDF/B-V
²⁴² Cm	Mughabghab	¹⁷⁸ Hf	Mughabghab	¹⁰² Pd	Mughabghab
²⁴³ Cm	Mughabghab	¹⁷⁹ Hf	Mughabghab	¹⁰⁴ Pd	Mughabghab
²⁴⁴ Cm	Mughabghab	¹⁸⁰ Hf	Mughabghab	¹⁰⁵ Pd	Mughabghab
²⁴⁵ Cm	Mughabghab	¹⁶⁵ Ho	Mughabghab	¹⁰⁶ Pd	Mughabghab
²⁴⁶ Cm	Mughabghab	¹²⁷ I	Mughabghab	¹⁰⁷ Pd	Mughabghab

¹⁰⁸ Pd	Mughabghab	⁷⁷ Se	Mughabghab	¹²⁴ Te	Mughabghab
¹¹⁰ Pd	Mughabghab	⁷⁸ Se	Mughabghab	¹²⁵ Te	Mughabghab
¹⁴⁷ Pm	Mughabghab	⁸⁰ Se	Mughabghab	¹²⁶ Te	Mughabghab
¹⁴⁸ Pm	Mughabghab	⁸² Se	Mughabghab	^{127^m} Te	Mughabghab
^{148^m} Pm	Mughabghab	Si	ENDF/B-V	¹²⁸ Te	Mughabghab
¹⁴⁹ Pm	Mughabghab	¹⁴⁴ Sm	Mughabghab	¹³⁰ Te	Mughabghab
¹⁴¹ Pr	Mughabghab	¹⁴⁷ Sm	Mughabghab	²³⁰ Th	Mughabghab
¹⁴² Pr	Mughabghab	¹⁴⁸ Sm	Mughabghab	²³² Th	ENDF/B-V
¹⁴³ Pr	Mughabghab	¹⁴⁹ Sm	Mughabghab	Ti	Mughabghab
²³⁸ Pu	Mughabghab	¹⁵⁰ Sm	Mughabghab	²³² U	Mughabghab
²³⁹ Pu	ENDF/B-V	¹⁵¹ Sm	Mughabghab	²³³ U	ENDF/B-VII Beta 2
²⁴⁰ Pu	JENDL 3.3	¹⁵² Sm	Mughabghab	²³⁴ U	Mughabghab
²⁴¹ Pu	ENDF/B-V	¹⁵³ Sm	Mughabghab	²³⁵ U	ENDF/B-V
²⁴² Pu	ENDF/B-V	¹⁵⁴ Sm	Mughabghab	²³⁶ U	Mughabghab
²⁴³ Pu	Mughabghab	¹¹² Sn	Mughabghab	²³⁷ U	Mughabghab
²⁴⁴ Pu	Mughabghab	¹¹⁴ Sn	Mughabghab	²³⁸ U	ENDF/B-V
⁸⁵ Rb	Mughabghab	¹¹⁵ Sn	Mughabghab	V	ENDF/B-V
⁸⁷ Rb	Mughabghab	¹¹⁶ Sn	Mughabghab	W	Mughabghab
¹⁸⁵ Re	ENDF/B-VI	¹¹⁷ Sn	Mughabghab	¹⁸² W	Mughabghab
¹⁸⁷ Re	ENDF/B-VI	¹¹⁸ Sn	Mughabghab	¹⁸³ W	Mughabghab
¹⁰³ Rh	Mughabghab	¹¹⁹ Sn	Mughabghab	¹⁸⁴ W	Mughabghab
¹⁰⁵ Rh	Mughabghab	¹²⁰ Sn	Mughabghab	¹⁸⁶ W	Mughabghab
⁹⁶ Ru	Mughabghab	¹²² Sn	Mughabghab	¹²⁴ Xe	Mughabghab
⁹⁹ Ru	Mughabghab	¹²⁴ Sn	Mughabghab	¹²⁶ Xe	Mughabghab
¹⁰⁰ Ru	Mughabghab	⁸⁴ Sr	Mughabghab	¹²⁸ Xe	Mughabghab
¹⁰¹ Ru	Mughabghab	⁸⁶ Sr	Mughabghab	¹²⁹ Xe	Mughabghab
¹⁰² Ru	Mughabghab	⁸⁷ Sr	Mughabghab	¹³⁰ Xe	Mughabghab
¹⁰⁴ Ru	Mughabghab	⁸⁸ Sr	Mughabghab	¹³¹ Xe	Mughabghab
¹⁰⁵ Ru	Mughabghab	⁸⁹ Sr	Mughabghab	¹³² Xe	Mughabghab
¹⁰⁶ Ru	Mughabghab	⁹⁰ Sr	Mughabghab	¹³³ Xe	Mughabghab
S	Mughabghab	¹⁸¹ Ta	Mughabghab	¹³⁴ Xe	Mughabghab
³² S	Mughabghab	¹⁸² Ta	Mughabghab	¹³⁵ Xe	Mughabghab
¹²¹ Sb	Mughabghab	¹⁵⁹ Tb	Mughabghab	¹³⁶ Xe	Mughabghab
¹²³ Sb	Mughabghab	¹⁶⁰ Tb	Mughabghab	⁸⁹ Y	ENDF/B-VI
¹²⁴ Sb	Mughabghab	⁹⁹ Tc	Mughabghab	⁹⁰ Y	Mughabghab
⁴⁵ Sc	ENDF/B-VI	¹²⁰ Te	Mughabghab	⁹¹ Y	Mughabghab
⁷⁴ Se	Mughabghab	¹²² Te	Mughabghab	Zr	Mughabghab
⁷⁶ Se	Mughabghab	¹²³ Te	Mughabghab	⁹⁰ Zr	Mughabghab

Appendix IV

List of nuclides with covariance information in 44GROUPV6REC set

Nuclide		Data source	Nuclide		Data source
¹⁰⁷ Ag	Mughabghab	²⁴⁸ Cm	Mughabghab	¹⁷⁷ Hf	Mughabghab
¹⁰⁹ Ag	Mughabghab	⁵⁹ Co	ENDF/B-VI	¹⁷⁸ Hf	Mughabghab
¹¹¹ Ag	Mughabghab	⁵⁰ Cr	ENDF/B-VI	¹⁷⁹ Hf	Mughabghab
²⁷ Al	ENDF/B-VI	⁵² Cr	ENDF/B-VI	¹⁸⁰ Hf	Mughabghab
²⁴¹ Am	ENDF/B-VI	⁵³ Cr	ENDF/B-VI	¹⁶⁵ Ho	Mughabghab
²⁴² Am	Mughabghab	⁵⁴ Cr	ENDF/B-VI	¹²⁷ I	Mughabghab
^{242m} Am	Mughabghab	¹³³ Cs	Mughabghab	¹²⁹ I	Mughabghab
²⁴³ Am	Mughabghab	¹³⁴ Cs	Mughabghab	¹³⁰ I	Mughabghab
⁷⁵ As	Mughabghab	¹³⁵ Cs	Mughabghab	¹³¹ I	Mughabghab
¹⁹⁷ Au	ENDF/B-VI	¹³⁷ Cs	Mughabghab	In	ENDF/B-VI
¹⁰ B	ENDF/B-V	⁶³ Cu	ENDF/B-VI	¹¹³ In	Mughabghab
¹¹ B	JENDL 3.3	⁶⁵ Cu	ENDF/B-VI	¹⁹¹ Ir	Mughabghab
¹³⁴ Ba	Mughabghab	¹⁶⁰ Dy	Mughabghab	¹⁹³ Ir	Mughabghab
¹³⁵ Ba	Mughabghab	¹⁶¹ Dy	Mughabghab	K	Mughabghab
¹³⁶ Ba	Mughabghab	¹⁶² Dy	Mughabghab	⁷⁸ Kr	Mughabghab
¹³⁷ Ba	Mughabghab	¹⁶³ Dy	Mughabghab	⁸⁰ Kr	Mughabghab
¹³⁸ Ba	Mughabghab	¹⁶⁴ Dy	Mughabghab	⁸² Kr	Mughabghab
¹⁴⁰ Ba	Mughabghab	¹⁶⁶ Er	Mughabghab	⁸³ Kr	Mughabghab
⁹ Be	Mughabghab	¹⁶⁷ Er	Mughabghab	⁸⁴ Kr	Mughabghab
Be-bound	Mughabghab	²⁵³ Es	Mughabghab	⁸⁵ Kr	Mughabghab
²⁰⁹ Bi	ENDF/B-VI	¹⁵¹ Eu	Mughabghab	⁸⁶ Kr	Mughabghab
²⁴⁹ Bk	Mughabghab	¹⁵² Eu	Mughabghab	¹³⁹ La	Mughabghab
⁷⁹ Br	Mughabghab	¹⁵³ Eu	Mughabghab	¹⁴⁰ La	Mughabghab
⁸¹ Br	Mughabghab	¹⁵⁴ Eu	Mughabghab	⁶ Li	Mughabghab
C	ENDF/B-VI	¹⁵⁵ Eu	Mughabghab	⁷ Li	ENDF/B-VI
C-graphite	ENDF/B-VI	¹⁹ F	ENDF/B-VI	¹⁷⁵ Lu	Mughabghab
Ca	Mughabghab	⁵⁴ Fe	ENDF/B-VI	¹⁷⁶ Lu	Mughabghab
Cd	Mughabghab	⁵⁶ Fe	ENDF/B-VI	Mg	Mughabghab
¹⁰⁶ Cd	Mughabghab	⁵⁷ Fe	ENDF/B-VI	⁵⁵ Mn	ENDF/B-VI
¹⁰⁸ Cd	Mughabghab	⁵⁸ Fe	ENDF/B-VI	Mo	Mughabghab
¹¹⁰ Cd	Mughabghab	Ga	Mughabghab	⁹⁴ Mo	Mughabghab
¹¹¹ Cd	Mughabghab	¹⁵² Gd	ENDF/B-VII Beta 2	⁹⁵ Mo	Mughabghab
¹¹² Cd	Mughabghab	¹⁵⁴ Gd	ENDF/B-VII Beta 2	⁹⁶ Mo	Mughabghab
¹¹³ Cd	Mughabghab	¹⁵⁵ Gd	ENDF/B-VII Beta 2	⁹⁷ Mo	Mughabghab
¹¹⁴ Cd	Mughabghab	¹⁵⁶ Gd	ENDF/B-VII Beta 2	¹⁴ N	Mughabghab
¹¹⁶ Cd	Mughabghab	¹⁵⁷ Gd	ENDF/B-VII Beta 2	¹⁵ N	Mughabghab
¹⁴⁰ Ce	Mughabghab	¹⁵⁸ Gd	ENDF/B-VII Beta 2	²³ Na	ENDF/B-VI
¹⁴¹ Ce	Mughabghab	¹⁶⁰ Gd	ENDF/B-VII Beta 2	⁹³ Nb	ENDF/B-VI
¹⁴² Ce	Mughabghab	⁷² Ge	Mughabghab	⁹⁴ Nb	Mughabghab
¹⁴³ Ce	Mughabghab	⁷³ Ge	Mughabghab	⁹⁵ Nb	Mughabghab
¹⁴⁴ Ce	Mughabghab	⁷⁴ Ge	Mughabghab	¹⁴² Nd	Mughabghab
²⁴⁹ Cf	Mughabghab	⁷⁶ Ge	Mughabghab	¹⁴³ Nd	Mughabghab
²⁵⁰ Cf	Mughabghab	¹ H	JENDL 3.3	¹⁴⁴ Nd	Mughabghab
²⁵¹ Cf	Mughabghab	H-ZrH	JENDL 3.3	¹⁴⁵ Nd	Mughabghab
²⁵² Cf	Mughabghab	H-poly	JENDL 3.3	¹⁴⁶ Nd	Mughabghab
²⁵³ Cf	Mughabghab	H-freegas	JENDL 3.3	¹⁴⁷ Nd	Mughabghab
Cl	Mughabghab	² H	CENDL 2	¹⁴⁸ Nd	Mughabghab
²⁴² Cm	Mughabghab	³ H	JEF 3.1	¹⁵⁰ Nd	Mughabghab
²⁴³ Cm	Mughabghab	³ He	CENDL 2	⁵⁸ Ni	ENDF/B-VI
²⁴⁴ Cm	Mughabghab	⁴ He	Mughabghab	⁶⁰ Ni	ENDF/B-VI
²⁴⁵ Cm	Mughabghab	Hf	Mughabghab	⁶¹ Ni	ENDF/B-VI
²⁴⁶ Cm	Mughabghab	¹⁷⁴ Hf	Mughabghab	⁶² Ni	ENDF/B-VI
²⁴⁷ Cm	Mughabghab	¹⁷⁶ Hf	Mughabghab	⁶⁴ Ni	ENDF/B-VI

²³⁷ Np	Mughabghab	¹⁰⁶ Ru	Mughabghab	¹⁶⁰ Tb	Mughabghab
²³⁸ Np	Mughabghab	S	Mughabghab	⁹⁹ Tc	Mughabghab
²³⁹ Np	Mughabghab	³² S	Mughabghab	¹²⁰ Te	Mughabghab
¹⁶ O	JENFL 3.3	¹²¹ Sb	Mughabghab	¹²² Te	Mughabghab
¹⁷ O	Mughabghab	¹²³ Sb	Mughabghab	¹²³ Te	Mughabghab
³¹ P	Mughabghab	¹²⁴ Sb	Mughabghab	¹²⁴ Te	Mughabghab
²³¹ Pa	Mughabghab	⁴⁵ Sc	ENDF/B-VI	¹²⁵ Te	Mughabghab
²³³ Pa	Mughabghab	⁷⁴ Se	Mughabghab	¹²⁶ Te	Mughabghab
²⁰⁶ Pb	ENDF/B-VI	⁷⁶ Se	Mughabghab	^{127^m} Te	Mughabghab
²⁰⁷ Pb	ENDF/B-VI	⁷⁷ Se	Mughabghab	¹²⁸ Te	Mughabghab
²⁰⁸ Pb	ENDF/B-VI	⁷⁸ Se	Mughabghab	¹³⁰ Te	Mughabghab
¹⁰² Pd	Mughabghab	⁸⁰ Se	Mughabghab	²³⁰ Th	Mughabghab
¹⁰⁴ Pd	Mughabghab	⁸² Se	Mughabghab	²³² Th	ENDF/B-VII Beta 2
¹⁰⁵ Pd	Mughabghab	Si	ENDF/B-VI	Ti	Mughabghab
¹⁰⁶ Pd	Mughabghab	²⁸ Si	ENDF/B-VI	²³² U	Mughabghab
¹⁰⁷ Pd	Mughabghab	²⁹ Si	ENDF/B-VI	²³³ U	ENDF/B-VII Beta 2
¹⁰⁸ Pd	Mughabghab	³⁰ Si	ENDF/B-VI	²³⁴ U	Mughabghab
¹¹⁰ Pd	Mughabghab	¹⁴⁴ Sm	Mughabghab	²³⁵ U	JENDL 3.3
¹⁴⁷ Pm	Mughabghab	¹⁴⁷ Sm	Mughabghab	²³⁶ U	Mughabghab
¹⁴⁸ Pm	Mughabghab	¹⁴⁸ Sm	Mughabghab	²³⁷ U	Mughabghab
^{148^m} Pm	Mughabghab	¹⁴⁹ Sm	Mughabghab	²³⁸ U	JENDL 3.3
¹⁴⁹ Pm	Mughabghab	¹⁵⁰ Sm	Mughabghab	V	ENDF/B-VI
¹⁴¹ Pr	Mughabghab	¹⁵¹ Sm	Mughabghab	W	Mughabghab
¹⁴² Pr	Mughabghab	¹⁵² Sm	Mughabghab	¹⁸² W	Mughabghab
¹⁴³ Pr	Mughabghab	¹⁵³ Sm	Mughabghab	¹⁸³ W	Mughabghab
²³⁸ Pu	Mughabghab	¹⁵⁴ Sm	Mughabghab	¹⁸⁴ W	Mughabghab
²³⁹ Pu	ENDF/B-V	¹¹² Sn	Mughabghab	¹⁸⁶ W	Mughabghab
²⁴⁰ Pu	JENDL 3.3	¹¹⁴ Sn	Mughabghab	¹²⁴ Xe	Mughabghab
²⁴¹ Pu	JENDL 3.3	¹¹⁵ Sn	Mughabghab	¹²⁶ Xe	Mughabghab
²⁴² Pu	ENDF/B-VI	¹¹⁶ Sn	Mughabghab	¹²⁸ Xe	Mughabghab
²⁴³ Pu	Mughabghab	¹¹⁷ Sn	Mughabghab	¹²⁹ Xe	Mughabghab
²⁴⁴ Pu	Mughabghab	¹¹⁸ Sn	Mughabghab	¹³⁰ Xe	Mughabghab
⁸⁵ Rb	Mughabghab	¹¹⁹ Sn	Mughabghab	¹³¹ Xe	Mughabghab
⁸⁷ Rb	Mughabghab	¹²⁰ Sn	Mughabghab	¹³² Xe	Mughabghab
¹⁸⁵ Re	ENDF/B-VI	¹²² Sn	Mughabghab	¹³³ Xe	Mughabghab
¹⁸⁷ Re	ENDF/B-VI	¹²⁴ Sn	Mughabghab	¹³⁴ Xe	Mughabghab
¹⁰³ Rh	Mughabghab	⁸⁴ Sr	Mughabghab	¹³⁵ Xe	Mughabghab
¹⁰⁵ Rh	Mughabghab	⁸⁶ Sr	Mughabghab	¹³⁶ Xe	Mughabghab
⁹⁶ Ru	Mughabghab	⁸⁷ Sr	Mughabghab	⁸⁹ Y	ENDF/B-VI
⁹⁹ Ru	Mughabghab	⁸⁸ Sr	Mughabghab	⁹⁰ Y	Mughabghab
¹⁰⁰ Ru	Mughabghab	⁸⁹ Sr	Mughabghab	⁹¹ Y	Mughabghab
¹⁰¹ Ru	Mughabghab	⁹⁰ Sr	Mughabghab	Zr	Mughabghab
¹⁰² Ru	Mughabghab	¹⁸¹ Ta	Mughabghab	⁹⁰ Zr	Mughabghab
¹⁰⁴ Ru	Mughabghab	¹⁸² Ta	Mughabghab		
¹⁰⁵ Ru	Mughabghab	¹⁵⁹ Tb	Mughabghab		

Appendix V

The 44-Group Structure

The 44-group structure is collapsed from a 238 fine-group structure. The broad-group boundaries subset was chosen for emphasizing the key spectral aspects of a typical LWR fuel package. Specifically, the broad-group structure was designed to accommodate the following features: two windows in the oxygen cross-section spectrum; a window in the cross section of iron; the Maxwellian peak in the thermal range; and the 0.3-eV resonance in ^{239}Pu . The resulting boundaries represent 22 fast and 22 thermal energy groups. The group structure upper energy boundaries are as follows:

Group	Upper E (eV) boundary
1	2.0000E+07
2	8.1873E+06
3	6.4340E+06
4	4.8000E+06
5	3.0000E+06
6	2.4790E+06
7	2.3540E+06
8	1.8500E+06
9	1.4000E+06
10	9.0000E+05
11	4.0000E+05
12	1.0000E+05
13	2.5000E+04
14	1.7000E+04
15	3.0000E+03
16	5.5000E+02
17	1.0000E+02
18	3.0000E+01
19	1.0000E+01
20	8.1000E+00
21	6.0000E+00
22	4.7500E+00
23	3.0000E+00
24	1.7700E+00
25	1.0000E+00
26	6.2500E-01
27	4.0000E-01
28	3.7500E-01
29	3.5000E-01
30	3.2500E-01
31	2.7500E-01
32	2.5000E-01
33	2.2500E-01
34	2.0000E-01
35	1.5000E-01
36	1.0000E-01
37	7.0000E-02
38	5.0000E-02
39	4.0000E-02
40	3.0000E-02
41	2.5300E-02
42	1.0000E-02
43	7.5000E-03
44	3.0000E-03
	1.0000E-05

Appendix VI

ANGELO and LAMBDA Description

INPUT DESCRIPTIONS FOR ANGELO-2.3 CODE

Ivo Kodeli and Enrico Sartori
NEA DATA BANK Version 2.3 (December 2007)

The purpose of this program is the expansion or collapsing of relative neutron cross section covariance matrices into a new energy group structure.

Read input parameters and options

record 1

Read TITLE (60 characters)

TITLE is general title of the library

record 2

Read IGO, IGM, NCAS, IBOX, NSW1, IPRT, MODE, IDEBUG (free format)

IGO	No. of groups in input matrix
IGM	No. of groups in output matrix
NCAS	No. of matrices to be processed
	=0 process all MTs found on COVERX file (for IBOX=1 only)
IBOX	=0 input library in BOXER format
	=1 input library in COVERX format
	=2 others (specified by NSW2 parameter)
NSW1	=0 lethargy boundaries in the input (IGO+1)
	=1 group boundaries in the input (IGO+1)
	=2 VITAMIN-J 175 group structure (built in)
IPRT	=0 minimum print option (recommended)
	#0 maximum print option (NOT TESTED)
MODE	mode of storage on output library
	=0 relative covariance/binary
	=1 standard deviations and relative covariance/binary
	=2 standard deviations and fractional correlations/binary
	=3 relative covariance in NJOY ERRORR format (recommended)
NLIB	=0 create a new library
	#0 append to the old library (if MODE=3 only)
IDEBUG	=0 do not print information useful for debug
	#0 print information useful for debug

record 3 :

Read MATD, ZA, (MT(i), i=1, NCAS) (free format)

MATD	material to be processed (use ENDF/B-6 standard)
ZA	1000*Z+A for principal scatterer
MT	reactions desired (all cross-correlations will be evaluated as well if found, otherwise set to 0. Not used if NCAS=0 & IBOX=1)

Notes:- Only one MATD/ZA can be read at a time.

- Either MATD or ZA should be provided (NOT BOTH), depending on what is used in the input library
- For IBOX=1 only: if NCAS=0 values of NCAS & MT are read from CVX file

records 4 and 5: Read input and output energy/lethargy grid

If (NSW1=1 and IBOX=2) Read (X(I), I=1, IGOPl)	input energy group structure in decreasing order (free format)
If (NSW1=1) Read (XF(I), I=1, IGMPl)	output energy group structure in decreasing order (free format)
If (NSW1=0 and IBOX=2)	

```

      Read (XOL(I),I=1,IGOP1) input lethargy group structure in increasing
                                order (free format)
      Read (XNL(I),I=1,IGMP1) output lethargy group structure in
increasing order(free format)

```

Omit the next records if (IBOX=0 or IBOX=1):

```

--->  Loop over all input matrices (NCAS)
      Read covariance information

Next two records
Read TITOLO Matrix Description (characters 80)
Read MATD,ZA,MT(i),MT1(i) (free format) (same as above)
Read BB,NSW2 (E12.6,I3)
      BB Threshold for zero setting (>0)
      If abs(value)<BB then value set to 0 (not used in this version)
      NSW2 Covariance information and format options

Next records
  if NSW2 =0  SYMMETRIC relative covariance matrix
              (only non-zero elements of the matrix should be provided)
              read n,m,COV(n,m) format(4(2I4,E10.2))
              COV is the relative covariance matrix (end with 0 0 0)
              COV(m,n) will be set equal to COV(n,m)
  if BSW2 =1  SYMMETRIC relative covariance matrix
              read (STD1(i),i=1,IGO) format(6F12.5)
              STD1 is relative standard deviation of reaction in %
              read n,m,CORR(n,m) format(6(2I3,F6.3))
              CORR is the correlation matrix (end with 0 0 0)
              (only non-zero elements of the matrix should be provided)
              CORR(m,n) will be set equal to CORR(n,m)
  if RSW2 =2  NON-SYMMETRIC relative covariance matrix
              read (STD1(i),i=1,IGO) format(6F12.5)
              read (STD2(i),i=1,IGO) format(6F12.5)
              STD1 is relative standard deviation of reaction 1 in %
              STD2 is relative standard deviation of reaction 2 in %
              read n,m,CORR(n,m) format(6(2I3,F6.3))
              CORR is the correlation matrix (end with 0 0 0)
              (only non-zero elements of the matrix should be provided)
  if NSW2 =3  SYMMETRIC relative covariance matrix
              read ((COV(n,m),n=1,IGO),m=1,IGO) free format
              full matrix must be provided
  if NSW2 =4  NON-SYMMETRIC relative covariance matrix
              read (STD1(i),i=1,IGO) free format
              read (STD2(i),i=1,IGO) free format
              STD1 is relative standard deviation of reaction 1 in %
              STD2 is relative standard deviation of reaction 2 in %
              read ((COV(n,m),n=1,IGO),m=1,IGO) format (6E13.6)
              full matrix must be provided
  if NSW2 =5  NON-SYMMETRIC relative covariance matrix
              read(STD1(i),i=1,IGO) free format
              read(STD2(i),i=1,IGO) free format
              STD1 is relative standard deviation of reaction 1 in %
              STD2 is relative standard deviation of reaction 2 in %
              read((CORR(n,m),n=1,IGO),m=1,IGO) free format
              full matrix must be provided

<-----continue loop NCAS times

      end of input description

```

ANGELO 2.3 OUTPUT TAPE DESCRIPTION

Output library is on logical unit 10 file called **LIB.NEW**

for MODE=0 to =2: output is written in binary form with the format:

1st part: file identification

record 1

TITLE (80 characters)

TITLE Library description (80 characters)

record 2

IGM, (XF(i), i=1, IGM+1), (XNL(i), i=1, IGM+1)

IGM No. of output groups

XF The energy group boundaries vector

XNL The lethargy group boundaries vector

2nd part:

---> Loop over all output matrices, as specified in input (NCAS)

Next record

N, MODE, IGM, TITOLO

N Covariance matrix sequence number

MODE Mode of storage (see input parameter RODE)

IGM No. of output groups

TITOLO Description of the matrix (80 characters)

Next record

if MODE =0 new interpolated relative covariance matrix
(IGM*IGM values)
=1 1st relative standard deviation (fractions)
2nd relative standard deviation (fractions)
relative covariance matrix (IGM*(IGM+2) values)
=2 1st relative standard deviation (fractions)
2nd relative standard deviation (fractions)
relative correlation matrix (IGM*(IGM+2) values)

<-----continue loop NCAS times

for MODE=3:

covariance matrices are written in the standard NJOY ERRORR format
(recommended).

INPUT DESCRIPTIONS FOR LAMBDA-2.3 CODE

Ivo Kodeli

NEA DATA BANK Version 2.3 (December 2007)

The purpose of this program is to check the mathematical properties of the multigroup covariance matrices. The correlation matrices are tested to determine if any element exceeds unity. The number of positive, negative, and zero eigenvalues is calculated and the matrix is classified on this basis. For LAMBDA the same input as for ANGELO 2.3 can be used.

Read input parameters and options

record 1

Read TITLE (60 characters)

TITLE is general title of the library

record 2

Read IGO, IGM, NCAS, IBOX (free format)

IGO No. of groups in input matrix

IGM Not used (enter 0)

NCAS No. of matrices to be processed

=0 test all data found in COVERX file (for IBOX=1 only)

IBOX =0 input library in BOXER format

=1 input library in COVERX format

record 3

Read MATD, ZA, (MT(i), i=1, NCAS) (free format)

MATD material to be processed (use ENDF/B-6 standard)

ZA 1000*Z+A for principal scatterer

MT reactions desired (all X-correlations will be evaluated as well if found, otherwise they will be set to 0).

Not used if (NCAS=0 and IBOX=1)

Notes: - only one MATD can be read at a time.

- either MATD or ZA should be provided but NOT BOTH, depending on what is used in the input library.

COVR MODULE OF NJOY99 CODE

Subroutine COVR

```

*****
*
* plot covariance data from errorr or make a condensed library.
*
* in the plot option, covr plots a matrix of correlation
* coefficients and an associated pair of standard deviation
* vectors, i.e. a covariance matrix. the correlation
* matrix is plotted as a shaded contour plot and the vectors
* are plotted as semi-log plots, one rotated by 90 degrees.
* the log energy grids for the vector plots are identical
* to the grids for the matrix plot. this version plots
* through viewr.
*
* in the library option, covr produces a condensed bcd
* covariance library in the boxer format. this format is
* efficient for matrices of simple blocks.
*
*---input specifications (free format)-----*
*
* card 1
*   nin          input tape unit
*   nout         output tape unit
*               (default=0=none)
*   nplot        viewr output unit
*               (default=0=none)
*
* ---cards 2, 2a, and 3a for nout.ne.0 only (plot option)
*
* card 2
*   icolor       select color or monochrome style
*               0=monochrome (uses cross hatching)
*               1=color background and contours
*               (default=0)
*
* card 2a
*   epmin        lowest energy of interest (default=0.)
*
* card 3a
*   irelco       type of covariances present on nin
*               0/1=absolute/relative covariances
*               (default=1)
*   ncase        no. cases to be run (maximum=40)
*               (default=1)
*   noleg        plot legend option
*               -1/0/1=legend for first subcase only/
*               legend for all plots/no legends
*               (default=0)
*   nstart       sequential figure number
*               0/n=not needed/first figure is figure n.
*               (default=1)
*   ndiv         no. of subdivisions of each of the
*               gray shades (default=1)
*
* ---cards 2b, 3b, and 3c for nout gt 0 (library option) only--*
*
* card 2b
*   matype       output library matrix option
*               3/4=covariances/correlations
*               (default=3)
*   ncase        no. cases to be run (maximum=40)
*               (default=1)
*
* card 3b
*   hlibid       up to 6 characters for identification
*
* card 3c
*   hdescr       up to 21 characters of descriptive
*               information
*
* ---cards 4 for both options---
*

```

```

* card 4
* mat desired mat number
* mt desired mt number
* mat1 desired mat1 number
* mt1 desired mt1 number
* (default for mt, mat1 and mt1 are 0,0,0
* meaning process all mts for this mat
* with mat1=mat)
* (neg. values for mt, mat1, and mt1 mean
* process all mts for this mat, except for
* the mt-numbers -mt, -mat1, and -mt1. in
* general, -n will strip both mt=1 and mt=n.
* -4 will strip mt=1, mt=3, and mt=4, and
* -62, for example, will strip mt=1, mt=62,
* mt=63, ... up to and incl. mt=90.)
* repeat card 4 ncase times
*
* note---if more than one material appears on the input tape,
* the mat numbers must be in ascending order.
*
*****

```

