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Innovative Methods

RESULTS OF THE IAEA CRP ON BENCHMARKS AGAINST EXPERIMENTAL DATA OF NEUTRONICS AND THERMALHYDRAULIC COMPUTATIONAL CODES FOR OPERATION AND SAFETY ANALYSIS OF RESEARCH REACTORS

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ABSTRACT

As one of the expected outputs of the Coordinated Research Project on “Innovative Methods in Research Reactor Analysis: Benchmark against Experimental Data on Neutronics and Thermalhydraulic Computational Methods and Tools for Operation and Safety Analysis of Research Reactors” (2008-2012), the IAEA will publish a technical document compiling the facility specifications, experiment descriptions and corresponding experiment data for a number of different RRs. Each data set was prepared in a way to serve as a stand-alone resource, allowing for the performance of independent benchmark exercises by interested institutions worldwide. The subject publication is in final preparation and compiles detailed facility descriptions and experiments covering a wide range of RR types, power levels and experimental configurations from 9 research reactors, namely ETRR-2 (22 MW, Egypt), IEA-R1 (5 MW, Brazil), MNR (3 MW, Canada), MINERVE (100 W, France), SRR-1/MNSR (30 kW, Syria), OPAL (20 MW, Australia), RSG-GAS (30 MW, Indonesia), SPERT-III (40 MW, USA), and SPERT-IV (variable power, Canada). Both neutronics and thermal-hydraulic experiments are available for benchmarking. In addition, the CRP will also provide an additional report on preliminary benchmark results and analyses with respect to available codes by the CRP participants, identify remaining open issues for future R&D activities, and indicate a possible role for the IAEA in the subject. It is understood that these publications will be helpful to improve operational performance and safety of research reactors. This paper will detail the above two publications in final preparation stage, including outline of the main benchmark results as reported in the last CRP related meeting, held in December 2012.

1. Introduction

Research reactors (RRs) are fundamental to the progress of both nuclear research and nuclear technology, and therefore the improvement of their design, performance and safety issues is of great importance. To deal with these challenges, computer codes allowing for better simulation of the complex processes and conditions in RRs have been developed. However, before utilizing these codes and methods, it is necessary to validate their model predictions and evaluate them in comparison with existing experimental data. This process is well known as benchmarking of computational tools against experimental data. But while a number of validated codes do exist for nuclear power plant simulations, there is a need to perform a similar qualification process in the case of RRs.

After a careful analysis of the present situation in the above context, a new Coordinated Research Project (CRP) on “Innovative Methods in Research Reactor Analysis: Benchmark against Experimental Data on Neutronics and Thermalhydraulic Computational Methods and Tools for Operation and Safety Analysis of Research Reactors” was designed and initiated in October 2008, as a cross-cutting activity jointly operated and equally funded by the three IAEA technical departments, namely NS, NE and NA [1]. The main objectives of this CRP [2] were to:

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- Encourage cooperation and foster exchange of information in the area of numerical analysis for improving RR design, operation and safety;
- Benchmark against experimental data the neutronics and thermal-hydraulic computational methods and tools used for operation and safety analysis of RRs, covering steady state and transient conditions;
- Stimulate the use and development of innovative RR modelling methods, and to support the transfer of such approaches to the larger RR community.

A group of close to 30 participants representing 16 Member States were engaged in this CRP to cover the above objectives. Participants from different countries (Fig. 1) with different background and development gathered in two groups, one as suppliers of experimental data, “Providers”, and the other one as the calculation group, the “Code-users”.



Figure 1: Geographical representation of the 16 countries formally involved in the subject CRP. Two additional countries, namely Brazil and Republic of Korea, participated and contributed as observers.

One of the main outcomes of this project is the 1st publication on “RR Benchmarking Database: facility description and experiments” that compiles the facility specifications, experiment descriptions and corresponding experimental data for 9 RRs, covering a wide range of RR types, power levels and experimental configurations. Each data set is prepared so as to serve as a stand-alone resource for independent benchmark exercises by interested institutions world-wide. The 2nd publication (in preparation) on “RR Benchmarking Results: code versus data comparison” will include benchmark results, analysis and interpretation from more than 20 participating institutions. Both documents are expected to be published by the IAEA in 2013, while their contents and partial results have already been reported in Ref. [3].

This paper will detail the above two publications in final preparation stage, including outline of the main consolidated benchmark results as reported in the last CRP related meeting, held in December 2012.

2. RR Benchmarking Database: facility description and experiments

As it is indicated in Table 1, data providers were responsible for submission of the description and necessary data of the facility to be benchmarked, including detailed RR specifications, experiment description and numerical experimental data. Comprehensive information on nine RRs of different powers and characteristics were collected for the

benchmark. Table 1 provides with the list of all these facilities including reactor name, country, reactor thermal power and type of fuel assembly.

Reactor (Country)	Power(MW)	Fuel Assembly
ETRR-2 (Egypt)	22	U3O8, flat plates
IEA-R1 (Brazil)	5	U3O8, flat plates
MINERVE (France)	0.001	UO2, fuel pins
MNR (Canada)	3	U3Si2, curved plates
MNSR (Syria)	0.03	UAl, thin rods
OPAL (Australia)	20	U3Si2, flat plates
RSG-GAS (Indonesia)	30	U3O8, flat plates
SPERT-III (USA)	40	UO2, rods
SPERT-IV (Canada)	Variable	UAl, flat plates

Table 1: List of RRs available for benchmarks within the CRP.

The spectrum of RR facilities is quite large, ranging from critical zero-power facilities (MINERVE) up to large power multipurpose reactors (RSG-GAS) and compact cores (OPAL). Moreover, fuel assemblies of different geometry and different reflector materials offers additional challenges for the calculation group (code-users).

The variety of experiments proposed by the providers (at least two per facility) also covered broad topics such as criticality, flux shape and profile, flux spectrum, control rod worth, reactivity effects and coefficients and kinetic parameters for the neutronic benchmarks while data for a loss of flow and for a reactivity insertion ramp were supplied for the thermalhydraulic comparison.

Reactor, country	Experimental data available	
	Neutronics	Thermalhydraulics
ETRR-2, Egypt	+	+
IEA-R1, Brazil	-	+
Minerve, France	+	-
MNR, Canada	+	-
MNSR, Syria	+	+
OPAL, Australia	+	-
RSG-GAS, Indonesia	-	+
SPERT III, USA	+	+
SPERT IV, Canada	+	+

Table 2: List of experiments (neutronics and thermalhydraulics) available for benchmarks within the CRP for different RRs types.

Such valuable diversity and amount of data allowed code-users to benchmark different neutronic tools and models and simulate postulated thermalhydraulic scenarios. In addition to well know commercial codes such as MCNP, PARET, RELAP and CATHARE, among others, a number of institution-developed codes (MERSAT, OSCAR, CONDOR, TRIPLOI,

etc.) were some of the tools used for the comparisons. Table 3 shows the participants and main computational tools employed in each case.

Country	Computational tools
Argentina	RELAP5
Australia	RELAP, PARET
Bangladesh	MCNP5, MVP, EUREKA-2
Canada	WIMS, REBUS, MCNP
France	TRIPOLI4, CATHARE2
Ghana	MCNP5, PARET, RELAP5, PLTEMP
Greece	RELAP5, PARET
Italy	WIMSD5, PARCS, RELAP5
Korea	MACARD, RELAP5
Nigeria	MCNP5, PARET
Romania	MCNP5, WIMS, CATHARE2
South Africa	OSCAR-4, MCNP5, RELAP5
Syria	MCNP5, MERSAT, RELAP5
USA	RELAP5, PARET

Table 3: List of computational tools used for the benchmarks by different CRP partners.

3. RR Benchmarking Results: code versus data comparison

The CRP provided a comprehensive set of data and some preliminary benchmark results clearly missing from literature. The postulated benchmark problems have been challenging and provided an excellent opportunity for share of information and good practices as long as validation of computational tools is concerned.

As it is detailed in Table 4, in most of the cases neutronics data include the reactor parameters such as core criticality (k_{eff}), neutron flux level/shape/profile, neutron flux energy distributions, control rod (CR) worth, reactivity effects, reactivity feedback coefficients and some kinetics parameters. Similarly, thermalhydraulics data include steady state (SS) temperatures and flow rate, loss of flow transients (LOFA), reactivity insertion transients (RIA) and other parameters.

Exp. data from	Neutronics							Thermalhydraulics		
	Criticality (K_{eff} , K_{inf})	Flux shape/profile	Flux spect.	CR worth	React. effects	Reactivity coeff.	Kinetic param.	SS	LOFA	RIA
OPAL	ARG, AUL, PAK, SAF, KOR					ARG, AUL, PAK, SAF				
ETRR-2	ARG, SAF							ARG, AUL, GRE, EGY, SYR, SAF		
MNSR-Y		PAK, SYR, USA+, GHA						Same		Same
Minerve	FRA, FRA2, ROM									
MNR	ARG, CAN, SYR, SAF			ARG, CAN, SYR, SAF						
RSG-GAS								ARG, GRE, EGY, SYR		
SPERT III	GHA,	GHA, ROM, USA								Same
SPERT IV	ALG, AUL, BGD, FRA, FRA2, PAK, SYR									Same
IEA-R1								ALG, ARG, BRAG RE, KOR, SYR, ITA, BGD		

Table 4: List of CRP partners signed up and performing benchmarks for various RR experiments.

The following briefly resumes some of the individual RR facilities benchmarked:

- OPAL (Australia): no major issues in this benchmark have been observed (e.g. see Fig.2) except some variation in the results obtained for control rod worth and kinetic parameters; specifications are of good quality and can serve for other teams as a good source for code benchmarking/qualification;
- MNR (Canada): some challenges in reproducing point kinetic parameters were identified; some of the benchmarks specifications need further clarifications and uncertainty in fuel burn-up specifications was found to be important in case of fresh versus used fuel core configurations;

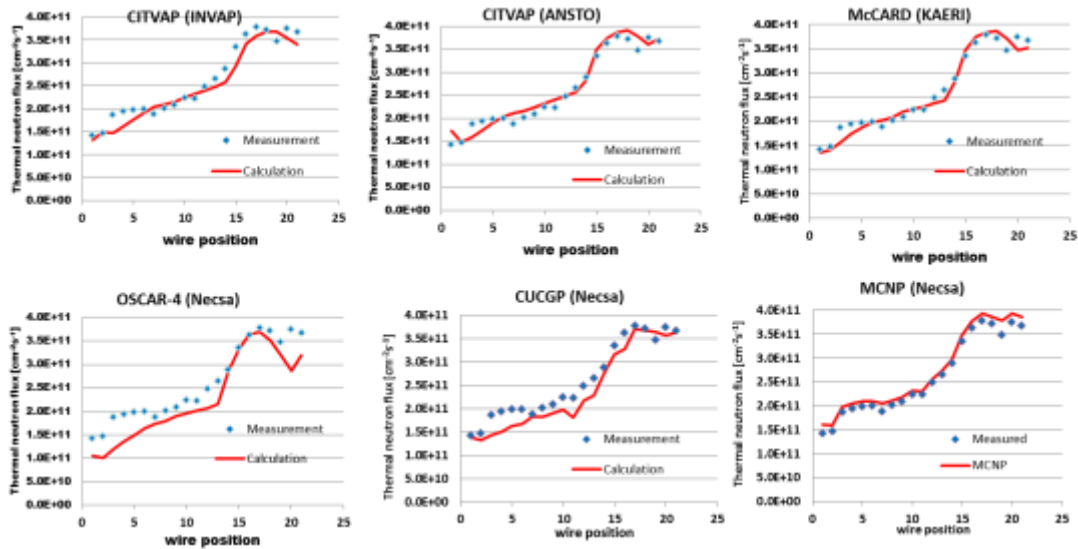


Figure 2: Steady state neutron flux profile for OPAL (Australia): experimental data is compared to different code/participant predictions.

- SPERT-IV D-Core: statics data/experiments are well qualified and had no major issues in reproducing them (e.g. see Fig.3); transient benchmarks are the most challenging; in this case large deviations and discrepancies have been observed between experiment and calculations and between the various calculations;

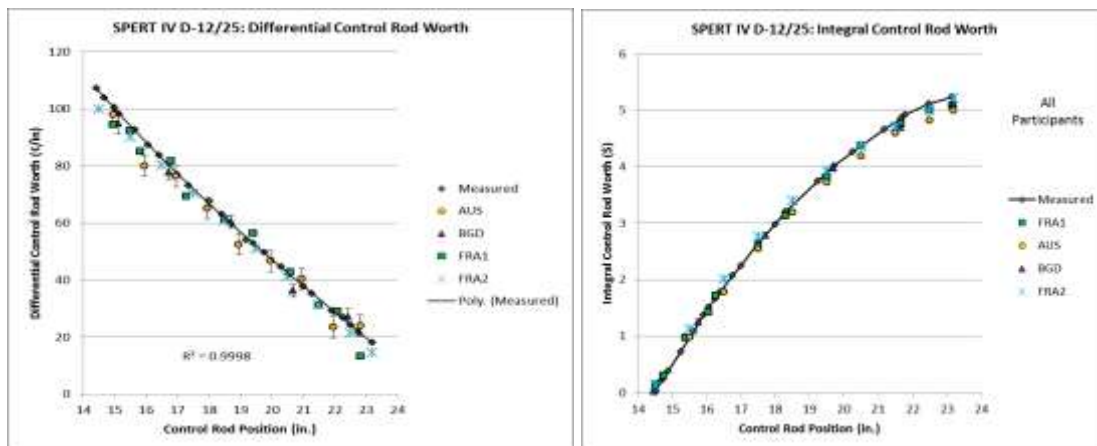


Figure 3: Comparison of experimental (black diamonds) and modelling results for SPERT-IV differential (on the left) and integral (on the right) control rod worth.

- ETRR-2 (Egypt) and RSG-GAS (Indonesia): overall data specifications are of acceptable quality; generally, keeping in mind conservatism, the results were of good quality (e.g. see Fig. 4); user effects were observed by comparing results produced by the same codes; in other cases, trends in the calculation results suggested limitations of some modelling tools; sharing of inputs decks was recommended to assist in identifying the cause of the observed variation, and perhaps initiate/support training;

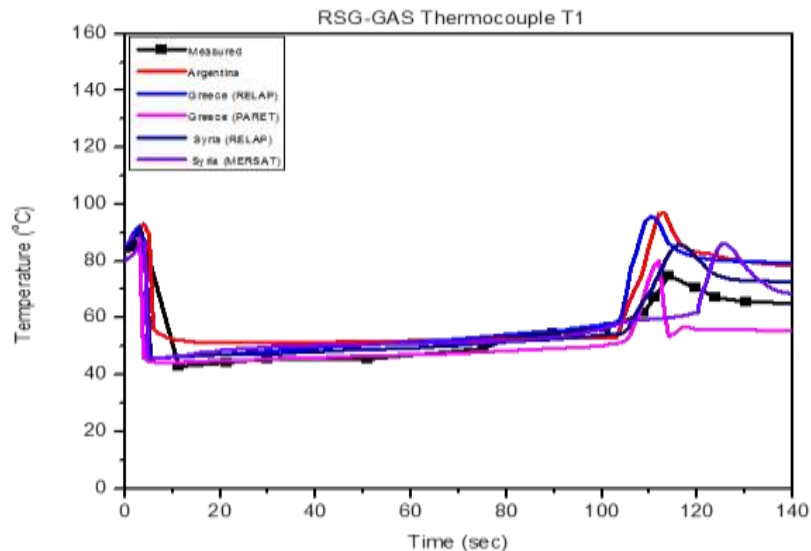


Figure 4: Comparison of Loss of Flow behaviour in RSG-GAS (Indonesia). Experimental data is presented in black-dotted line. The 1st peak corresponds to the RR scram, while the 2nd peak to the flow reversal.

- MINERVE (France): overall definition and availability of uncertainties regarding specifications are of high importance and will be helpful in interpreting results; available predictions were of good quality; need for verification of dependence of results on nuclear data libraries was identified;
- MNSR-Y & IEA-R1: the data and experiments are of acceptable quality; from the available benchmarks it was concluded that some code modifications might be required to include improved correlations and 3D effects; it was recommended to continue the efforts beyond this CRP; clear user effects were observed using RELAP5 code (e.g. see Fig. 5); therefore share/comparison of input decks was strongly recommended.

As reported during the last CRP meeting, held in December 2012 in Vienna (Austria), preliminary benchmark analysis performed so far has highlighted a number of important findings:

- The various benchmark problems have been challenging and have provided an excellent opportunity for good practice and lessons learned. Although the CRP has achieved a great deal in gathering relevant benchmarks and performing preliminary analysis on all of these, it was noted that interactions between neutronics and thermal-hydraulics components of these benchmarks were still not optimal. In most cases these disciplines were treated rather independently and suggestions for improvement include either coupled calculations, or at least coupled approaches by neutronic and thermal-hydraulic analysts;

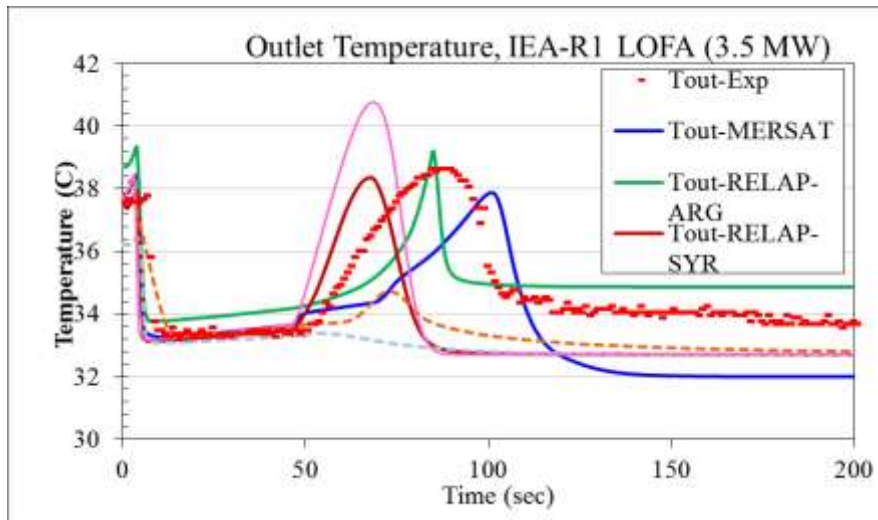


Figure 5: Comparison of Loss of Flow behaviour in IEA-R1 (Brazil). Experimental data is presented in red-dotted line. The 1st peak corresponds to the RR scram, while the 2nd peak to the flow reversal.

- Benchmark development, followed by fine detail and fine scale modelling took significant effort and justified extension of the CRP for an additional year. However, there is a need to continue dedicated communication efforts between participants and relevant data providers, including code developers when possible;
- The comparison planned within this CRP between individual submissions by the participants and joint benchmarking efforts is an added value of this project in terms of evaluating both user effects and models used in the codes employed. In the analysis of submitted results, when possible, a clear distinction should be made between the evaluation of the code versus the evaluation of the user effect. In addition, feedback to code developers in the process will be also valuable. Therefore, continuation of joint activities after closure of this CRP is advisable;
- The benchmarks performed so far show that neutronics modelling has proven to be reasonably accurate; obtaining good agreement for thermal-hydraulics analysis is more challenging as similar problems were experienced by many of the users.
- It would be useful to continue the benchmarking process. Interested participants were welcomed to share their updated results in a dedicated meeting. IAEA is committed to organize and host such a technical meeting following participants' request;
- The definition of quality of the benchmarks is a difficult task, and often shortcomings are only found during advanced stages of the modelling. Nevertheless the supplied benchmarks have reached an acceptable level of completeness and certainly add significant value to the RR community;
- Good communication between data suppliers, analysts, and code developers should be continued and facilitated. For example, some input decks will be shared among the analysts and the code developers for cross check and advice as necessary.

4. Summary

As a result of this CRP a great amount of the experimental data was obtained from different CRP participants, covering a wide range of RR types, power levels and experimental configurations. It includes 9 different RR facilities. It is understood that this database makes a considerable contribution to the benchmarking and validation of neutronics and thermal-hydraulic computational methods and tools that are used for the operation and safety analysis of RRs in different Member States. It will also encourage cooperation and foster exchange of information in the area of numerical analysis for improving RR design, operation

and safety among interested institutions, both within the CRP participants as well as other stakeholders. Within the scope of this CRP a number of participants have also supplied their benchmark results based on these provided specifications, which will be published separately. These analyses have greatly contributed to the verification and quality of this benchmark database.

Based on the feedback and subject to the availability of new experimental data, it is planned that the RR benchmarking data base will be updated with other RR specifications and experimental data. It is also envisioned that a series of training workshops will be organized bringing interested parties in benchmarking and validation of the modeling tools against the variety experimental data available thanks to this CRP. In addition, it is planned that a dedicated web portal will be created and maintained for follow up activities to support the present CRP community as well as other interested parties in terms of knowledge management, sharing of experiences and good practices in benchmarking of RRs as well as use of various modelling tools. Last but not the least, the CRP partners recommended the IAEA to define and initiate a new CRP on RR based depletion benchmarks, that would address the issues related to efficient reactor fuel utilization, source term definition, waste quantification, irradiation of various targets and other topics of interest for safety and utilisation of RRs. This new CRP is scheduled to start in 2014.

5. Acknowledgements

The authors of this paper would like to acknowledge contribution and cooperation to all partners of the IAEA CRP 1496 [2], with special thanks and appreciation to the data providers and results consolidators.

6. References

[1] D. Ridikas, et al., “The IAEA Activities Related to Reactor Physics under Sub-programme Research Reactors”, Proceedings of the ANS Winter Meeting, San Diego, CA, USA, 11-15 Nov. 2012; ANS Transactions Vol. 107 (2012).

[2] The IAEA CRP 1496 on “Innovative Methods in Research Reactor Analysis: Benchmark against Experimental Data on Neutronics and Thermalhydraulic Computational Methods and Tools for Operation and Safety Analysis of Research Reactors” (2008-2012); more information on the subject CRP can be found at http://www-naweb.iaea.org/napc/physics/research_reactors/crps/crp.html (last accessed in March 2013).

[3] A. Doval, et al. “The IAEA Coordinated Research Project on Benchmarking of Research Reactor Experiments from Ten Facilities World-wide”, Proceedings of the ANS Winter Meeting, San Diego, CA, USA, 11-15 Nov. 2012; ANS Transactions Vol. 107 (2012).

OPERATIONAL NEUTRONIC ANALYSIS FOR QUALIFICATION OF IRRADIATION EXPERIMENTS AIMED TO TEST LEU HIGH DENSITY FUEL AT BR2 HIGH FLUX MATERIALS TESTING REACTOR

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ABSTRACT

Since more than a decade new high density LEU fuel assemblies and plates are irradiated in the BR2 reactor aimed to evaluate the fuel performance at high neutron and high heat fluxes. Several types of baskets, containing assemblies with various plates can be loaded in different channels. The qualification process requires fulfilling strictly and reliably the design irradiation conditions in each plate for the evolution of the average/peaking power density and fuel burn-ups at the hot spot, during the whole irradiation cycle. To satisfy the requested irradiation scenario, optimization calculations include provisional simulation of several irradiation cycles for different reactor core environment. Pre-irradiation and post-irradiation calculations, performed before/after each irradiation cycle, include amendment of the core environment and comparison with available post-irradiation measurements of neutron fluxes and fuel burn-up. At BR2 we use a sophisticated calculation model including MCNP and SCALE modules with post processing simulation of detailed 3-D core burn-up evolution. The post processing module calculates the evolution of the fuel burn-up in a mesh in each plate for several time steps during each cycle. The results for such irradiations are presented in the paper.

1. Introduction

The development of high-density LEU fuels has made an important progress in the last years. In particular, the qualification of the dispersed UMo fuel system with densities up to ~ 7.5 - 8.5 gU_{tot}/cm³ is making substantial progress although irradiation tests at very high heat-fluxes still are to be performed.

BR2 is actively involved in the qualification process of high-density (~8 gU_{tot}/cc) LEU fuel. The irradiation concerns full-size high density U7Mo experimental plates and annular fuel elements containing Al or Al+Si matrix with ²³⁵U enrichment, equal to 19.7%. The plates and annular fuel elements containing LEU plates have been manufactured by AREVA-CERCA.

The core of the BR2 reactor contains 79 channels: 64 standard channels (Ø84.2 mm), 10 reflector channels (Ø50 mm) and 5 large channels (Ø200 mm). Each channel has a hexagonal Be reflector, which is inclined by its own angle so, that in each cross section of the core, at the Z-plane, a triangular water gap exists between the channels formed by the hexagonal Be matrix. The variable BR2 core typically contains 30-34 drive fuel elements and the remaining channels are loaded with large dedicated irradiation assemblies or small fission targets for radioisotopes production. Dedicated irradiations can continue several cycles during which the fuel depletion (burn-up) significantly is changing

Most of the irradiation experiments for qualification of LEU plates are accompanied by:

- Activation foils measurements of the Westcott conventional thermal neutron flux and of the equivalent fission flux in reactor channels;
- Non-destructive measurements of fission events distribution in the irradiated fuel plates;
- Destructive radiochemical analysis of the sample cut from irradiated fuel plates.

The operational control of the irradiation conditions inside the dedicated experiments is performed by monitored online coolant temperature measurements, by online measurements of neutron and gamma fluxes using self-powered fission and gamma detectors. All these measurements provide possibility to control irradiation conditions and to verify (validate) the computer model of BR2 which is used for provisional and for post-irradiation calculation analysis.

2. BR2 computer Model

Provisional optimization analysis is used to find the conditions which satisfy the rated irradiation requirements for the dedicated experiments, to determine the interference between the neighbor reactor channels. Post-irradiation re-calculations of the operating cycle are based on consideration of the actual operating history of the BR2 (including possible scram events) and the actual reloading scheme of the uranium fission targets in the reactor core during the cycle.

For reliable simulation of the irradiation history in the dedicated device, the BR2 computation model must include as much as possible detailed and accurate description of the status of the whole reactor core, such as:

- Exact geometrical description of all devices in the core and in the reflector.
- Detailed spatial and isotopic fuel burn-up distribution in the whole reactor core. The number of different fuel zones used for simulation of the fuel burn-up distribution in the drive BR2 fuel elements is about 1000. About several thousand depletion zones are used for the modeling of the dedicated fuel assemblies.
- The spatial distribution and the time evolution of ^3He in the Be matrix during the reactor shut-down and during the operation cycle are also taken into account.
- Provisional positions of control rods during the cycle history.
- Dedicated computer software algorithm is used for Post-processing of MCNP-SCALE output results to obtain the data required for simulation of the spatial and time evolution of the fuel burn-up and poisoning products in the drive fuel elements.

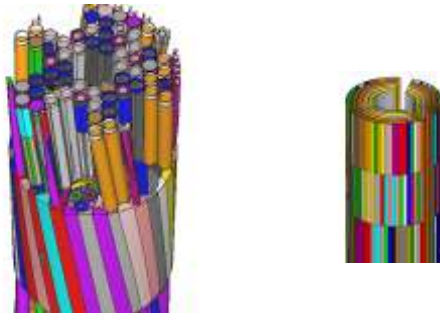


Fig 1. Schematic view of the BR2 inclined channels and BR2 fuel plates with the burn-up registration mesh.

The contemporary computer codes permit to simulate most of the physical processes in the reactor core by using dedicated software codes. In most cases, transfer of output information from one computer code to another code as input data, requires special efforts to prepare dedicated input files. Automatic transfer of output results from one code to another usually requires dedicated linking modules.

Accurate prediction of the fuel burn-up distribution and of the change of fissile nuclides concentration in the fuel element is important for maintaining the requested power and irradiation conditions in the tested fuel elements. However, it is time consuming to perform a direct calculation of the detailed fuel burn-up distributions using the Monte Carlo codes in fine meshes in each fuel element irradiated in different positions in the reactor core. In practice, the mean fuel burn-up in the fuel elements is calculated using the neutron fluxes

and reaction rates averaged over several fuel zones inside the fuel element. Such simplified approach permits to predict accurately the irradiation history of the fuel elements in the reactor core. However, detailed information about the spatial distribution of the fuel burn-up in the fuel plates requires more qualified (sophisticated) approach.

Routinely used computer codes for fuel management and for neutronic analysis of each BR2 cycles are: MCNP-4C[1] and SCALE-4.4a [2], and their later versions MCNP-5, MCNPX, SCALE-6. The basic BR2 model uses MCNP and/or MCNPX (with switched off automatic burn-up module). Each fuel assembly (flat or multi-plate annular cylindrical) includes the computational mesh. Each cell of the meshes has unique material compositions. This permits to simulate accurately the spatial fuel burn-up distributions and the time evolution after changing of the burn-up in each cell.

The dedicated interface module automatically adapts the MCNP input file for the next time step by changing the spatial burn-up distributions in the mesh cells inside all dedicated fuel assemblies and in the BR2 fuel elements using the calculation results of the previous time step (distributions of power, fluxes) and the data-base of fuel burn-up evolution. The burn-up data-base includes the evolution of the fuel burn-up composition versus the released energy and the duration of shutdown periods in the provisional irradiation history. These data are prepared in advance with the help of the SCALE code.

The adaptation of the fuel burn-up in the MCNP input data in the BR2 driver fuel elements and in the dedicated fuel assemblies for the next time step, takes a few seconds of the computer processing time, which is considerably faster compared to the computing time of the automatic burn-up modules integrated into the neutron transport codes, such as MCNPX 2.7.0 or SCALE-6.

2.1 Calculation of fuel burn-up distribution

The burn-up of the fissile nuclide atomic number density during the operating cycle can be approximated using the standard assumptions for a constant reactor power over 'depletion time step' in the calculation algorithm. The fuel burn-up history and the change of the fuel composition in the local fuel zone can be calculated using the mean values of the burn-up in the fuel element (or rod, or plate) and the power peaking factor distributions. For this purpose, regular meshes of registration cells, $\{v\}_n$ $\{n=1, N\}$, are created in fuel elements in order to avoid different statistical errors in cells. The dependence of the fuel burn-up, $\beta(v, T)$, expressed as the ratio of burned fissile atoms in the registration cell $\{v\}_n$ to their initial concentration versus the energy released in a fuel zone at the end of a depletion time T is determined as:

$$\beta(v, T) = C_v \frac{\int_0^T P(v, t) dt}{M(v)} 100\%, \quad C_v = \frac{A_U}{N_A E_{eff}} \alpha_v, \quad \alpha_v = \frac{\langle \sigma_f + \sigma_c \rangle_v}{\langle \sigma_f \rangle_v}$$

where A_U is the atomic mass number of the fissile element, N_A is the Avogadro constant, E_{eff} is the effective fission energy, $M(v)$ is the weight of the fuel in the cell $\{v\}$ in the beginning of the irradiation period and $P(v, t)$ is the power at the time t . Writing the similar equations for the mean burn-up in the whole fuel element, we can express the dependence of the local burn-up $\beta_v(T_N)$ as function of the mean burn-up, $\bar{\beta}(T_N)$, in the fuel rod, and the change of the specific power peaking factors $k_v(T_i)$, after the N^{th} irradiation time step during the irradiation.

The functional dependence of the fuel burn-up, $\beta(v, t)$, in the registration cell $\{v\}$ on the mean burn-up $\beta_{FE}(T)$ in the fuel element, and on the specific power peaking factor $k_v(T)$ at time t , can be obtained as:

$$\beta(v, T) = k_v(T) \bar{\beta}_{FE}(T) \frac{\alpha_v}{\alpha_{FE}}, \quad k_v(T) = \frac{P(v, T)}{M(v)} \frac{M_{tot}}{P_{FE}(T)}$$

where $P(v, T)$ and $P_{FE}(T)$ are the time-integrated powers in the particular fuel zone at the position $\{v\}$ and in the whole fuel element (plate), respectively. The function $k_v(T)$ is a specific power peaking factor, which is determined using the power distribution in the mesh $\{v\}$ inside each fuel element. The ratio $\alpha_v/\alpha_{FE}=1$ for the fuel element containing one type of fissile composition in all fuel plates.

After N irradiation time steps (the duration of the N^{th} step is denoted as T_N) the local fuel burn-up, $\beta_v(T_N)$ in each fuel zone $\{v\}$ can be calculated as:

$$\beta_v(T_N) = \beta_v(T_1) + \sum_{i=2}^N (\bar{\beta}(T_i) - \bar{\beta}(T_{i-1})) \times \kappa_v(T_i) = \sum_{i=1}^{N-1} \bar{\beta}(T_i) [\kappa_v(T_i) - \kappa_v(T_{i+1})] + \beta(T_N) \kappa_v(T_i),$$

$$k_v(T_N) = \frac{\int_{T_{N-1}}^{T_N} P(v, t) dt}{M(v)} \frac{M_{tot}}{\int_{T_{N-1}}^{T_N} \int_V P(v, t) dt dv}$$

The mean fuel burn-up in the whole fuel rod (element) can be calculated for the mean operation power using the SCALE or ORIGEN codes. The dependence of the nuclide composition versus the energy deposition (or, equivalently, versus the fuel burn-up) in the fuel rod (element) can be calculated only once and be kept in the form of a burn-up data bank. These data are used each time when it is necessary to extract the fuel composition for the local burn-up in the registration mesh.

In the approach presented here, it is not necessary to solve the burn-up equation in each registration zone. It is only necessary to calculate the detailed distribution of the power peaking factors on the registration mesh. After that the distributions of the power peaking factors, k_v , are used to obtain the distributions of the fuel burn-up in registration cells. The nuclide composition in the registration cell for the evaluated fuel burn-up can be extracted from the burn-up data bank, which contains the dependence of the fuel composition on the fuel burn-up (or release energy).

The distribution of fission events in the mesh can be evaluated using the fuel burn-up distributions, atom concentrations and the effective fission rate for ^{235}U and ^{239}Pu in the cells of the mesh inside a dedicated fuel assembly.

The burn-up of ^{235}U in the HEU and LEU at small burn-up in practice linearly depends on the released fission energy in the fuel. At high burn-up of ^{235}U in the LEU fuel, the deformation of the linear dependence, due to the breeding of ^{239}Pu , is not very strong, Fig.2 (a). The fraction of ^{239}Pu nuclides in the LEU fuel remains less than 5% relatively to ^{235}U , for burn-up of ^{235}U up to 50%, Fig.2 (b) At the very high burn-up of ^{235}U ($> 80\%$), the mass of ^{239}Pu reaches 10-15% relatively to the mass of ^{235}U . At the ^{235}U burn-up of 60%, the fission rate of ^{239}Pu is faster than ^{239}Pu breeding, Fig.2 (c).

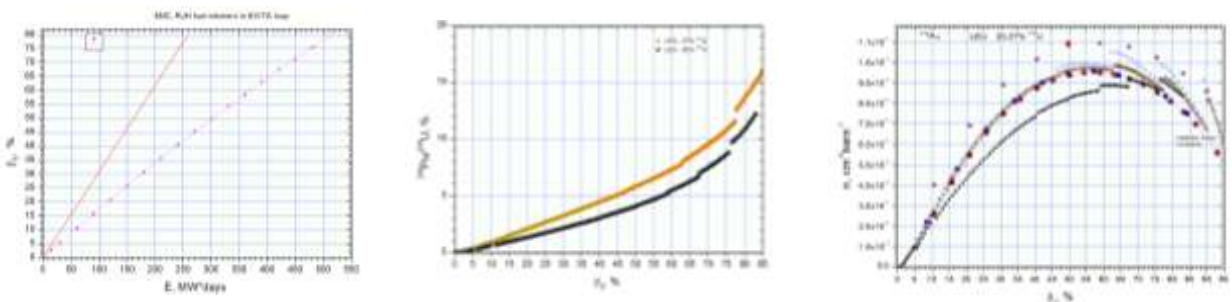
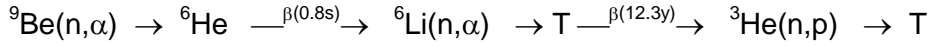


Fig.2 (a) Burnup of ^{235}U in HEU and in LEU fuel, (b) ratio of ^{239}Pu to ^{235}U in LEU fuel plates and (c) evolution of ^{239}Pu in LEU of different enrichment between irradiation cycles versus the ^{235}U burnup.

2.2 Poisoning of Be matrix

The poisoning of beryllium is a process, which is caused by neutron absorption of all energies in Be. The poisoning effect starts on the threshold (n, α) reaction on ${}^9\text{Be}$, irradiated by fast neutrons with energy $E_n > 0.69$ MeV and following transmutations into nuclides of ${}^6\text{Li}$, ${}^3\text{He}$ and T:



The ${}^6\text{Li}$ and ${}^3\text{He}$ isotopes have very high absorption cross section of thermal neutrons and their accumulation in the Be-matrix depend on the reactor power history and the position of the channel. After some time of the reactor operation the concentration of ${}^6\text{Li}$ reaches saturation. During the reactor operation ${}^3\text{He}$ is burning out and the ${}^3\text{H}$ concentration increases with the fission energy produced. After the shut down of the reactor, the concentrations of ${}^3\text{He}$ increases due to the decay of T, thereby causing reactivity losses of the reactor core. For example, Be material is used as a reflector & moderator in several reactors: BR2, MARIA[3], WWR-M...

Example of changing ${}^3\text{He}$ content in different channels during several irradiation cycles and during shut-downs is depicted in Fig.3.

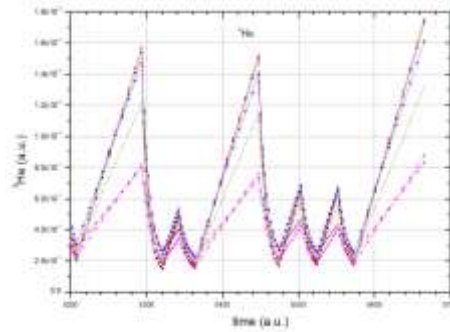


Fig.3. Time evolution of ${}^3\text{He}$ concentration in different Be channels during BR2 irradiation cycles and shut-downs.

3 Activation dosimetry analysis for irradiation of LEU plates

The dedicated E-FUTURE irradiation basket (see fig. in Table 1) can include 4 different large size fuel plates. The central holder plate in the basket is designed to receive wires which include activation dosimeters for measurements of thermal and fast neutron fluxes. Usually ${}^{59}\text{Co}$ and Ag, ${}^{54}\text{Mn}$ activation dosimeters are used to measure Westcott's thermal neutron flux, Φ_0 , and the epithermal flux Φ_{epi} using the results of the measured reaction rates [4]:

$$R_{\text{Co}} = \sigma_0^{\text{Co}}(E_0)\Phi_0 + I_{\text{res}}^{\text{Co}}\Phi_{\text{epi}}; \quad R_{\text{Ag}} = \sigma_0^{\text{Ag}}(E_0)\Phi_0 + I_{\text{res}}^{\text{Ag}}\Phi_{\text{epi}};$$

The Westcott conventional flux of thermal neutrons, Φ_0 , has been defined as a ratio of the reaction rate R_i to the cross-section $\sigma_{n,\gamma}^{\text{Co}59}(E_0)$, where the cross-section $\sigma_{n,\gamma}^{\text{Co}59}(E_0) = 37.18$ barns is defined at the energy $E_0 = 0.0253$ eV.

$$\varphi_0(r_i) = \frac{R_i}{\sigma_{n,\gamma}^{\text{Co}59}(E_0)}. \quad \varphi_0(r_i) = \nu_0 \int_0^{0.5\text{eV}} \frac{\varphi(r_i, E)}{\nu} dE, \quad R_i = \int_0^{E_{th}} \sigma_{n,\gamma}^{\text{Co}59}(E)\varphi(r_i, E)dE,$$

where $\nu_0 = 2200$ m/s; ν is the neutron velocity and the integral defines the total number of neutrons in the thermal energy range; E_{th} is the upper boundary of energy for thermal neutrons; $\sigma_{n,\gamma}^{\text{Co}59}(E)$ is the activation cross-section for ${}^{59}\text{Co}$ in (n, γ) reaction; r_i is the position

of the dosimeter; $\varphi(r_i, E)$ is the neutron flux density in the foil, normalized to the nominal reactor power.

Generally, the Westcott conventional flux is lower than the thermal neutron fluence rate by the factor of difference between the mean velocity of the neutron spectrum and the most probable velocity in the thermal neutron spectrum. Moreover, the temperature dependence of the thermal neutrons spectrum may influence the Westcott conventional flux.

The measured 'equivalent fission flux' is evaluated from the ^{54}Mn activity : $^{54}\text{Fe}(n,p)^{54}\text{Mn}$ [4]:

$$\varphi_\chi = \int_0^{20} \sigma_{np}^{Fe54}(E) \varphi(E) dE / \langle \sigma_{np}^{Fe54} \rangle, \quad \langle \sigma_{np}^{Fe54} \rangle = 0.0801 \text{ b},$$

The calculated 'equivalent fission flux' is calculated as

$$\varphi_{fiss} = \int \sigma_{np}^{Fe54}(E) \varphi(E) dE / \int \sigma_{np}^{Fe54}(E) \chi(E) dE$$

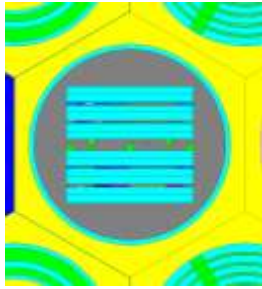
where $\chi(E)$ is the fission spectrum for ^{235}U . The measured 'equivalent fission flux' is different from the definition of fast neutron fluence rate ($E > 1\text{MeV}$). The ratio of the fast neutron fluence rate ($E > 1\text{MeV}$) to the 'equivalent fission flux' depends on the distance between the irradiation point and the source of fission neutrons. In the case of BR2 this ratio varies from 0.85 to 1.1.

Activation measurements were performed during three BR2 cycles aimed to control the irradiation of LEU fuel plates in the E-FUTURE basket. The positions of the activation dosimeters in the central holder of the basket are shown as the projection to the fuel plate (red ellipses) in Fig. 4. Three wires, each containing four sets of (Co, Al, Fe) needles at different axial position were irradiated during different times in 3 cycles:

- The wire in position W1 was irradiated during the first 2 cycles, and then the new wire was loaded for irradiation in cycle #5 (see Table 2).
- The wire in position W2 was irradiated during all 3 cycles.
- The new wire in position W3 was planned to be irradiated during each cycle. Due to technical problems, activation dosimeters in one of the axial positions, in W3, were lost after the first cycle. In the next cycle the whole wire W3 was lost. Finally, in the last cycle, the irradiations and the analysis were finished as planned.

The results of the measurements and of the post irradiation re-calculation of the actual irradiation history in each position of the activation needles are presented in Table 2 as a difference between measurements and calculations. All results represent the mean effective Westcott's conventional thermal neutron flux averaged of the duration of 1, 2, or 3 cycles. The lost data represent 21% from the total number activation needles. For 67%-71% of the activation needles, a difference of 3%-8% between the calculations and the measurements was found. The remaining 8%-12% of the needles had the average difference of about 20% due to unreliable information about actual axial position of the lost activation needles in the wire W3 during the first irradiation cycle. In the case of the lost needle W3 (b) (see Table 3), the maximum error was 7%, but if the needles was in another position as in the case W3(a), the maximum error in this wire during cycle #3 would be equal to 19%.

The reliability of the predictions in the presented comparison can be estimated using the data in Table 3. Technical problems occurred in 21% of the activation needles. For the remaining 67-71% of the dosimeters, the difference between the predictions and measurements was in the range of 3-8%. Only in two (or three) axial positions at the bottom of the channel the difference was equal to 20%-30%. This difference is caused probably by manipulations inside the neighboring channel containing a dedicated basket with fission targets.



Cycle #	Wire W1	Wire W2	Wire W3
3			1 position lost
4			lost
5			

Table 1. Positions of Wires with activation Dosimeters in the E-Future irradiation basket and the schedule of wire activation during cycles.

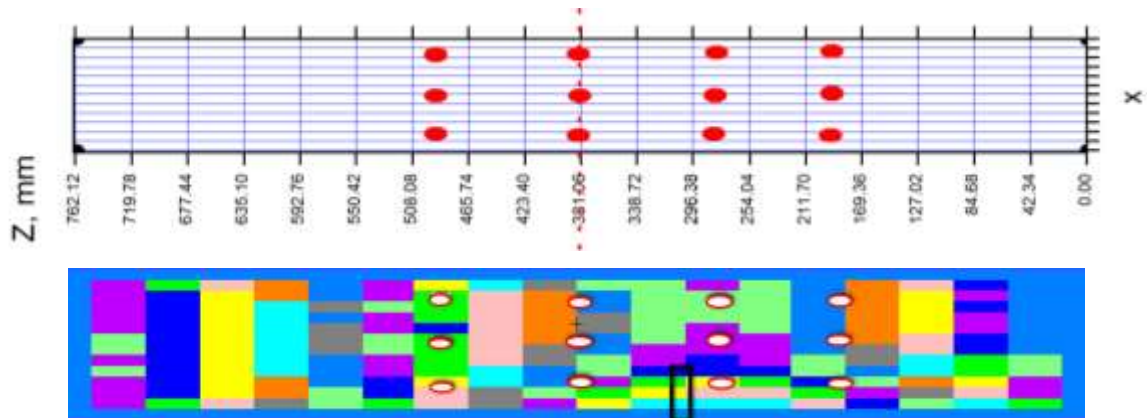


Fig. 4 Schematic presentation of the activation dosimeters projections onto the LEU fuel plate with the mesh (upper fig). The position of the destructive cut for radiochemical analysis and the material mesh is shown on the lower figure.

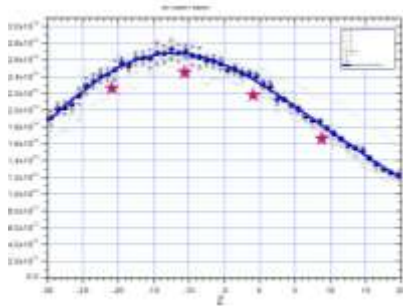
Cycle	W1	W2	W3(a)	W(b)
3	8 % 9 %		2 %	2 %
			10 %	<i>lost</i>
			19 %	0 %
			<i>Lost</i>	-7 %
4	8 % 9 %	-8 % -6 % -6 % +22 %	<i>lost</i>	<i>lost</i>
			<i>lost</i>	<i>lost</i>
			<i>lost</i>	<i>lost</i>
			<i>lost</i>	<i>lost</i>
5	3 % 3 % 3 % 29 %		3 %	
			3 %	
			4 %	
			6 %	

Table 2. Difference between the calculated and the measured average Westcott's conventional thermal neutron flux: each wire contains 4 sets of activation needles at different axial positions.

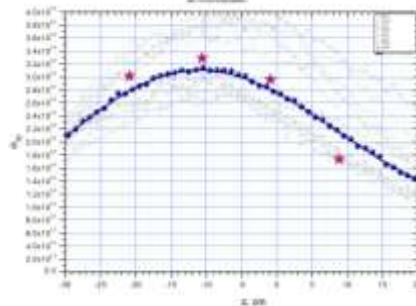
Fraction of Dosimeters,%	Difference calculation / measurements, %
71-67	3-8
8-12	20-30
21	No data

Table 3. Reliability of predictions.

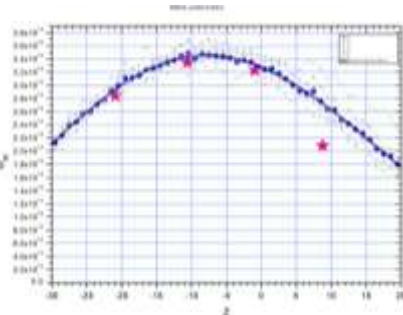
W1 (Cycles 3-4)



W2 (cycles 3-4-5)



W1 (cycle 5)



W3 (cycle 5)

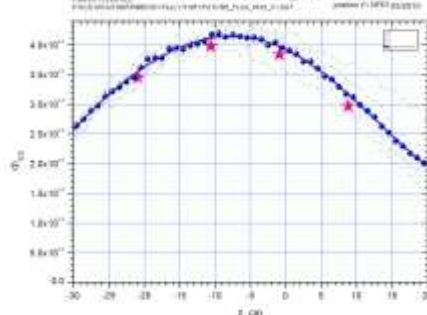


Fig.5 Axial distribution of the average Westcott convention thermal neutron flux measured during several cycles in different positions near LEU high density fuel plates in the E-Future basket. Blue curves are obtained from post-irradiation re-calculation of the actual irradiation history, and the red stars are the results of the activation needles measurements.

4 Activation dosimetry measurements of the time evolution of the thermal neutron flux

Additional comparisons were performed for the measured time evolution of the Westcott thermal neutron flux in the dedicated channel. The measurements are performed by BR2 staff (P.Claes, K.Verstreepen) every 2 days using activation foils. For reliability the measurement are performed 2 times using 2 foils. The flux value is accepted if the difference between these 2 measurements is less than 2% error. As can be seen from Fig.6, the provisional evolution of the thermal flux correlates with the actual activation measurements within the accuracy of 2-3%. The difference of 2-3% between the provisional and the measured evolution can be important in precise irradiations, but is it less important for the most experiments of LEU irradiations.

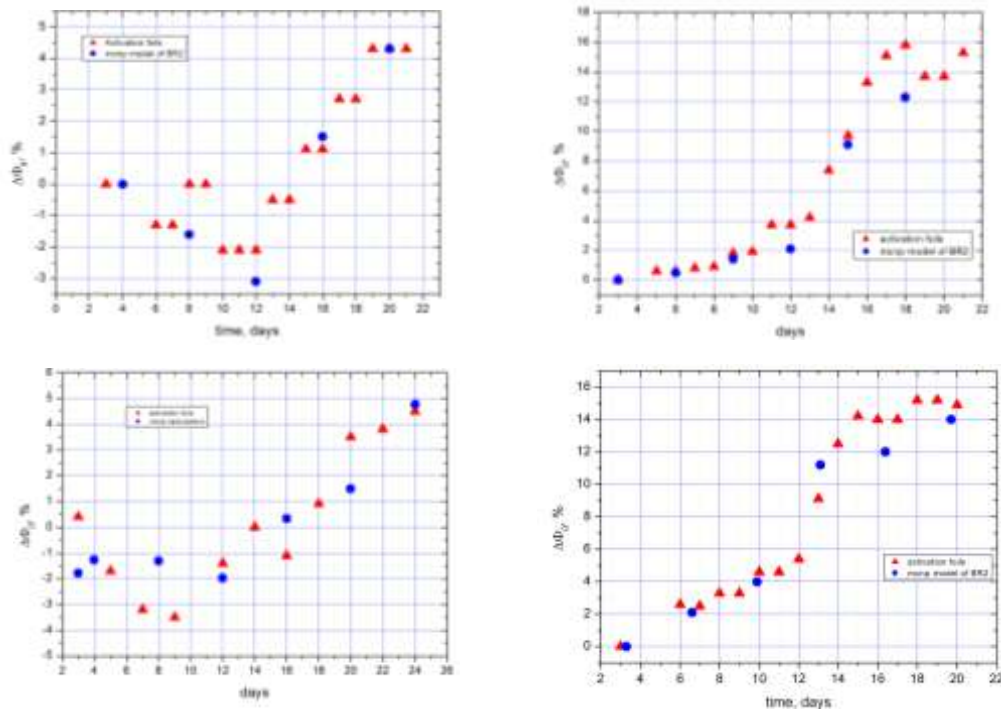


Fig.6 Time evolution of the Westcott thermal neutron flux in four cycles. Activation foils measurements are marked by the red triangles (the change of flux is not corrected between the measurements). The predicted evolutions is given in % relatively to the start of analysis (blue circles) and were calculated before the reactor start-up in each of the 4 cycles in 2012.

5 Radiochemical determination of the burnup in UMo FUTURE fuel plate

Destructive radiochemical analysis of the UMo plate (19.8% ^{235}U) irradiated at different conditions (lower heat fluxes) and time, was performed in SCK-CEN by M.Gysemans et. al [5]. The measurement of FIMA (Fissions per Initial Metal Atom) was performed in the sample which was cut from the irradiated plate in the position situated near the hot plane. This place is marked in Fig. 4 by the black rectangle.

The initial content of ^{235}U in the fresh UMo was equal to 19.82%, i.e. the fuel contains 249.4 mg ^{235}U per 1000 mg ^{238}U (^{234}U and ^{236}U are considered separately).

Provisional calculations for the evolution of the spatial burn-up distribution in the plate during irradiation were performed using the SCALE & MCNP model of BR2. At the ^{235}U burn-up of $\beta_5=29.7\%$, the ^{239}Pu content is 2.1% relatively to ^{235}U , which is in a very good correlation with the measurements (see below results of the radiochemical measurements). The calculation mesh in the plate was different from the size of the sample cut. The burn-up calculation of ^{235}U in the region close to the sample cut position is 27.0% of the fission events of ^{235}U , which is 31%-32% from the total burn-up of ^{235}U .

In the radiochemical measurements, performed by M.Gysemans et. al, the weight of ^{235}U per 1g of ^{238}U has been evaluated: it was equal to 0.176 g $^{235}\text{U}/1\text{g}$ ^{238}U . The content of ^{239}Pu at the end of the irradiation was equal to 2.1% relatively to the weight of ^{235}U . The burnup of ^{235}U in the analysed sample was about 29.4%.

Radiochemical determination of FIMA was based on measurements using ^{137}Cs , ^{144}Ce , ^{143}Nd , ^{150}Nd monitors. The measured values were equal to 4.97%-5.09%. The average value was equal to 5.06% \pm 0.008% FIMA. The difference between the calculation predictions and

the radiochemical analysis is was about 0.3 %FIMA. The analytical calculations based on the MCNP model gave ~27% of the burned ²³⁵U in fission events in the place of the sample location versus 25.25% by the radiochemical analysis.

	²³⁵ U burn-up, %	%FIMA	Fissions ²³⁵ U
Radiochemical analysis	29.4	5.06	25.25%
Provisional Calculations, MCNP-SCALE model of BR2	31-32	5.35	27.0%

Table 4. Results of Radiochemical determination of the burn-up and of the computer simulation.

6 Conclusions

The control on the irradiated-flat and incurved large fuel plates, containing high density UMo LEU fuel under the rated maximum heat fluxes of 470-500 W/cm² in the hot spot, is managed combining computer simulations using a sophisticated BR2 model qualified by measurements of neutron fluxes. The computer model of BR2 is built using the MCNP and SCALE codes, including an additional dedicated post-processing module for simulation of the evolution of the spatial fuel burn-up distributions in the fuel plates and assemblies. Routinely, the calculated provisional irradiation conditions are verified by comparing with the available activation dosimeters data, non-destructive and destructive radiochemical analysis of the fuel burn-up. Using online measurements of the coolant temperature in the thermal balance approach, the measured power is compared with the calculated deposited power in dedicated reactor channels. Multiple comparisons confirm that the accuracy in the prediction of the irradiation conditions in BR2 by described computer model is within ±10%. The measurements of the Westcott thermal neutron fluxes by activation dosimeters during irradiation of four LEU high density UMo fuel plates coincide with calculated fluxes within error margin of 3-8% for 90% of available dosimeters. The other 10% of dosimeters have larger deviation of 20-30% due to manipulations inside the neighbour channel used for radio-isotope productions. Destructive radio-chemical analysis of the fuel burn-up in UMo plate irradiated at lower heat fluxes differs from the calculation results by 0.3%FIMA, and by 5-8% for the number of fission events in ²³⁵U. The predicted time evolution of the thermal neutron flux in the dedicated irradiation channels usually differs from the activation dosimeters measurements by 2-3%.

Acknowledgement We are grateful to our colleagues V.Willekens, P.Claes, K.Verstreepen for the results obtained from the analysis of activation foils and needles irradiated in BR2 reactor.

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ITU TRIGA MARK II RESEARCH REACTOR: A BENCHMARK ANALYSIS WITH VARIOUS CODES

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ABSTRACT

The main purposes of research reactors are to make miscellaneous training and research, to irradiate materials to be tested, to produce radioisotopes for industrial/medical applications and to make neutronic analysis including pulse experiments under very high neutron density. In addition, the research reactors would readily provide invaluable knowledge on testing and validation of the codes. The reliability of the codes would depend on how the outcomes are in harmony with the experiments. Since such reactors consist of a great deal of complexity in components with various dimensions such as water gaps, irradiation channels, control rods, graphite reflector, etc., simplifications (e.g., assuming an equally distributed fuel mass in all fuel rods) play a significant role in modelling to influence the calculation sensitivity. For this purpose, up to present, various codes, primarily Monte Carlo method and Discrete Ordinate methods, have been utilized for the validation based on a particular design of research reactors. However, the comparison of the codes has not been yet clearly presented for this type of reactors.

In this manner this study deals with the validity of various radiation-transport codes, utilising different methods, in ITU TRIGA Mark II reactor. The codes to be used in modelling of the reactor are selected to be MCNP5, SERPENTv1.17 along with updates, TRIGLAV linked with WIMSD5B code, and DRAGON3.06K. It is also focused during the study on the neutron criticality analysis when the reactor operates at cold zero-power. On the other hand, in the analyses only ENDF/B-VII.0 is used for the state-of-art neutron cross-section libraries of isotopes to eliminate its influence. The criticality analyses and neutron flux calculations throughout the core are carried out in the bank and withdrawn position of the control rods. Furthermore, the reactivity worth of control rods is presented. Finally, this study would be likely to fill the gap of the literature in this area and would give some promising code-by-code benchmarking results in support of better modelling of the research reactors.

1. Introduction

It is possible to model a physical system in many ways using any reactor physics code. It is also clear that the number of modelling increases as the different codes are used. In here, the critical issue about the models to be used is the reliability of the codes and the agreement between the code results and the experimental data. The advantageous of the code-by-code benchmarking is to offer an opportunity to observe the validity of the codes and also is to bring to light the deficiencies, errors and issues related with the codes (and also originated from the user) in the course of modelling.

There are several studies reported in the literature: a comparison between the codes is made by Yang et al. [1] for TRIGA reactor at university of Utah using four different codes. In the mentioned study, research reactor has modelled in 2-D using AGENT code and the results are compared with well-known Monte Carlo methods. The other comparison was made by Keller [2] for the OSTR (Oregon State University TRIGA Reactor) using Attila code.

In this study, the focus is modelling the ITU TRIGA Mark II by using various radiation transport codes which uses different solution methods. The codes used in modelling of the reactor are selected to be MCNP5, SERPENT, TRIGLAV linked with WIMSD5B code, and DRAGON3.06K. Neutron criticality analyses are performed when the reactor operates at cold zero-power. ENDF/B-VII.0 is used for the state-of-art neutron cross-section libraries of isotopes to eliminate its influence. The criticality analyses and neutron flux calculations for the core are carried out for the bank and withdrawn positions of the control rods. Finally, the reactivity worth of control rods is presented.

2. Used Codes, Reactor Parameters and Methodology

2.1 Used Codes

MCNP5 [3] is a Monte Carlo radiation transport code that solves three dimensional configuration of materials in geometric cells for neutron, photon, and electron particles using continuous or discrete energies.

SERPENT [4] is a three-dimensional continuous-energy Monte Carlo reactor physics burnup calculation code. The code uses an analogue Monte Carlo method to simulate a self-sustaining chain reaction for neutron transport ray-tracing and the Woodcock delta-tracking method. Since it uses continuous-energy cross sections (in ACE format), the code is capable of simulating other neutron interaction types (i.e., low energy interaction and free-gas scattering).

TRIGLAV code [5] is used for TRIGA Mark II reactor to compute power and flux distributions and fuel element burnup. Using two-dimensional time-independent diffusion equation in radial and azimuthal directions of cylindrical geometry, finite difference equations is solved simultaneously. Group constants (e.g., diffusion coefficients) for each considered unit cell such as fuel element and graphite dummy are generated by WIMSD5B.

DRAGON code [6] can simulate a unit cell or a fuel assembly in two/three-dimensional geometry. Neutron transport equation can be solved by using method of characteristics and collision probability method according to the problem type.

2.2 Reactor Description

ITU TRIGA Mark II Reactor was started to operate in 1978 at the Energy Institute of İstanbul Technical University for the purpose of training the students, performing experiments related with the nuclear reactor physics applications and producing radioisotopes for industrial/medical applications. It is cooled by light water and the core is placed into the pool that has a height of 6.40 m and a diameter of 2 m. The reactor uses 69 fuel elements with 20% U-235 enriched $\text{UZrH}_{1.6}$ fuel. In addition, the reactor includes one thermal column and three beam ports.

ITU TRIGA MARK II Reactor core map is presented in Fig 1. The core is made up of fuel elements (FE, IFE, GR), control rods (RR, SR, TR), a source hole, a central thimble and a pneumatic irradiation channel. The core with radius of 21.81 cm is surrounded by a block of cylindrical graphite reflector with a thickness of 29.83 cm. Length of fuel region of fuel element is 38.1 cm while the total length of the fuel element is about 73 cm. Three control rods are filled with B_4C absorber material and the absorber material is enclosed with stainless steel cladding thickness. Control rods move inside the aluminium tubes.

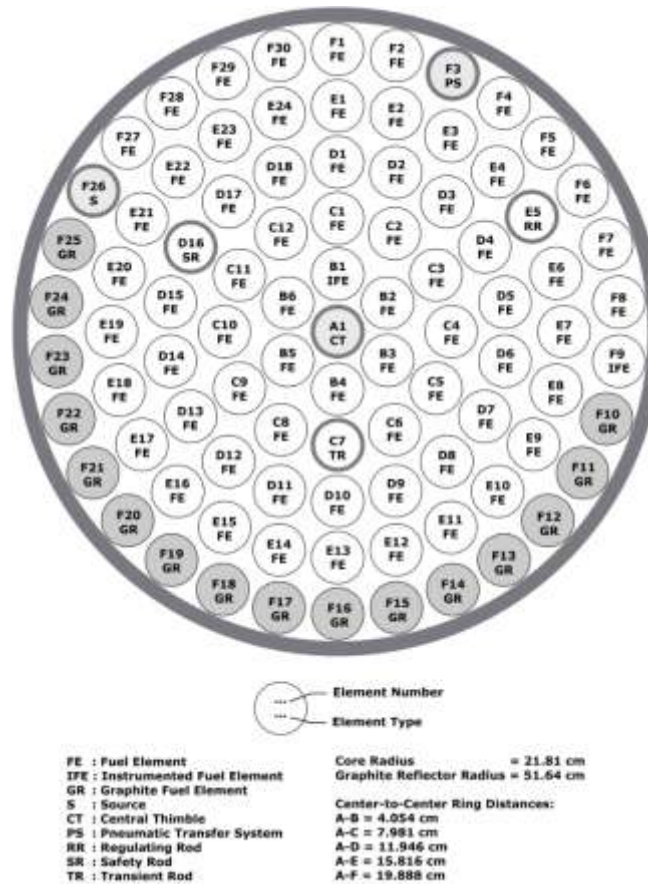


Fig 1. ITU TRIGA Mark II Reactor Core Map

2.3 The methods used in modelling

MCNP5 and SERPENT inputs are prepared for 3-D geometry in details. Number of neutron history is set to 15 000 000 with 1500 cycle in both codes. The calculational error in relative unit is less than 0.00020 for MCNP5 and 0.00035 for SERPENT model. Due to the lack of zirconium in hydrogen libraries in the SERPENT code, effect of thermal scattering is not properly modelled. Monte Carlo models include beam ports and thermal column.

In TRIGLAV code, the leakage as buckling is set to $4.52 \times 10^{-3} \text{ cm}^{-2}$. According to the log book of ITU TRIGA Mark II reactor operation, the excess reactivity of the fresh core configuration at a power of 250 kW is 1057 pcm. The same buckling is used in the model prepared for the DRAGON code. In addition, the core is modelled with ring shaped graphite block and water region outside the graphite block.

TRIGLAV input is prepared for 2-D geometry in r- θ directions. Method of characteristic with S_{32} is used in DRAGON code model to solve the two-dimensional transport equation. Due to large number of region and complex geometry configuration of TRIGA core in 3-D, the DRAGON input is prepared for 2-D. The computation is performed with some modifications in cells. For instance, very small cells and their material contents are merged with adjacent cells by preserving total volume and mass contents.

While continuous energy ENDF/B-VII.0 [7] neutron cross-section library is used in MCNP5 and SERPENT model, 172 group ENDF/B-VII.0 WLUP library [8] updated by IAEA is used in TRIGLAV and DRAGON calculations. Water temperature is assumed to be constant as 295 K. $S(\alpha, \beta)$ libraries for H in ZrH_2 and Zr in ZrH_2 is taken into account only for MCNP5.

3. Results

According to the results listed in Table 1, multiplication factors agree very well with the experimental data when the control rods are in critical and withdrawn positions. Only

deterministic codes deviate slightly from the experiment due to inaccurate modelling of the reactor, for example, some particular geometries such as control rods with aluminium tubes are not adequately introduced into the TRIGLAV code. Also, some contributions to the disparity come from the selected solution method.

Table 1 Comparison of core multiplication factor (k_{eff})

	Critic	Withdrawn
Experimental	1.00	1.0460
MCNP5*	1.00134	1.04603
SERPENT2	1.00213	1.04609
TRIGLAV5	-	1.04673
DRAGON3.06K	-	1.04651

Normalized flux distribution in relative units throughout the core region in radial direction is showed in Fig 2. The left side of the figure shows MCNP5 results and the other side presents the results of SERPENT calculations. Case (a) illustrates the distribution of fast neutron flux and case (b) is for thermal flux. As seen from the plots, results of SERPENT are fairly well in agreement with that of MCNP5 code. It is evident that the fast flux reaches its highest value within the fuel region of fuel rods. Towards the center of the core, level of the fast flux increases stepwise and gets the highest value at the inner ring. In case of thermal flux, it reaches its local maximum value within the water boxes. The highest value is obtained in the central thimble. SERPENT results, as a whole, get along with that of MCNP5, although the some values slightly differs.

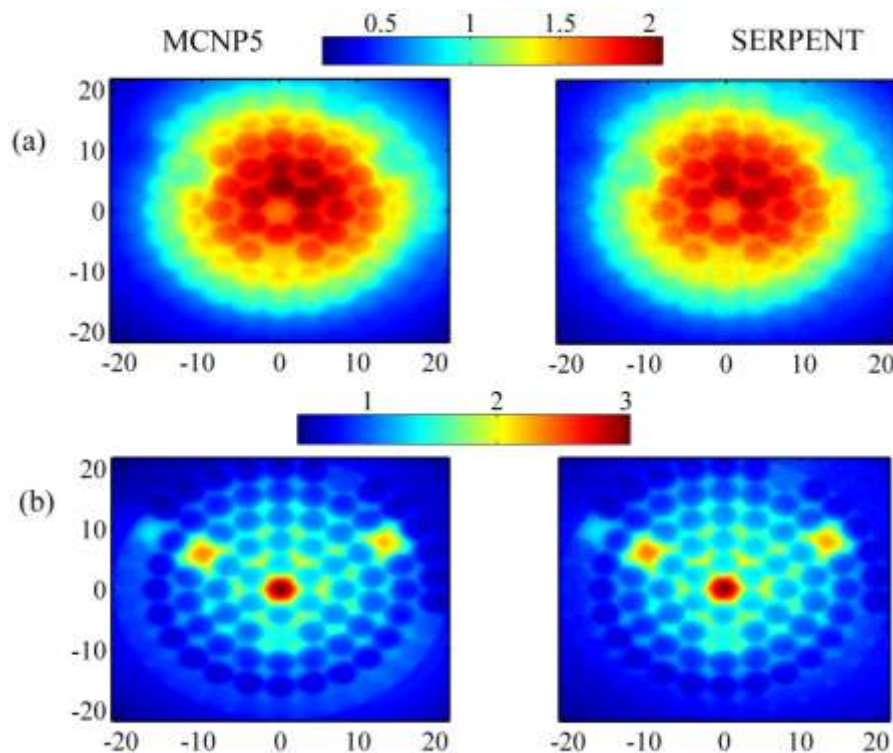


Fig 2 Normalized flux distribution throughout the core

Core power peaking factors are shown in Fig 3. The capital letters between the lines refer to ring name displayed in Fig 1 and the fuel element number is increased by one starting from the fuel element number B1. From the results, MCNP5 and SERPENT yield more or less the same values. However, TRIGLAV code gives somewhat different results from the Monte Carlo methods at the fuel elements near the regions that are filled with water. The difference comes from inaccurate modelling of the control rods, irradiation tube and neutron source holes. In these regions, well-thermalized neutron flux (as clearly seen in Fig 2) affects the neighbourhood fuel elements.

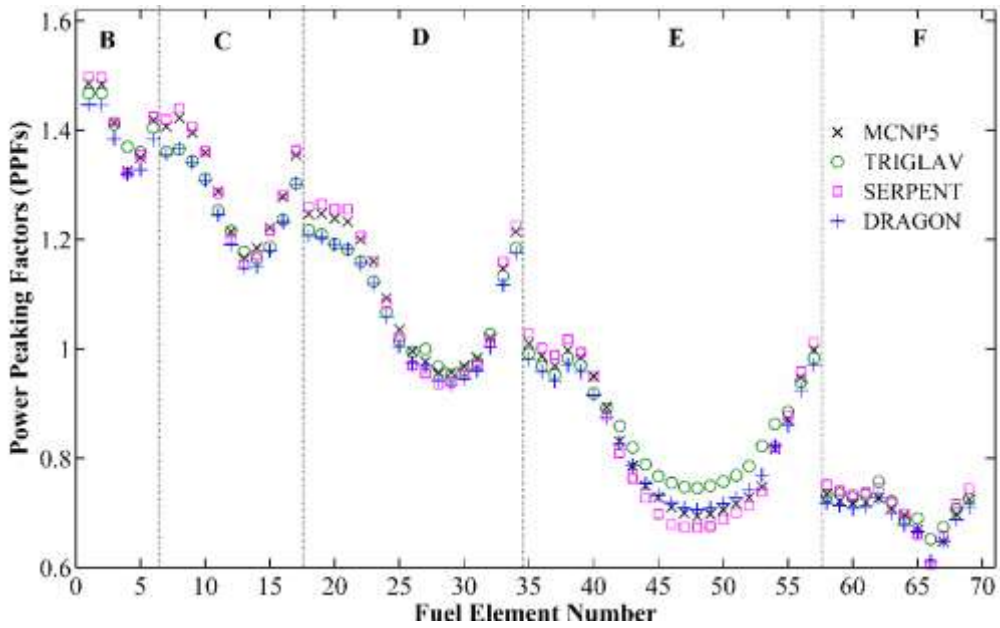


Fig 3. Power peaking factors

Reactivity worth of control rods for MCNP5 and SERPENT codes are given in Fig 4. As seen from the figures, each code reaches the same total reactivity that can be inserted to the reactor core and agrees very well with the experimental data. In addition, the reactivity worth curves obtained from the codes completely overlaps with the experimental curve for transient and regulating rods. On the other hand, experimental data curve of the safety rod is not accurately calculated, although the MCNP5 and SERPENT codes give the same results.

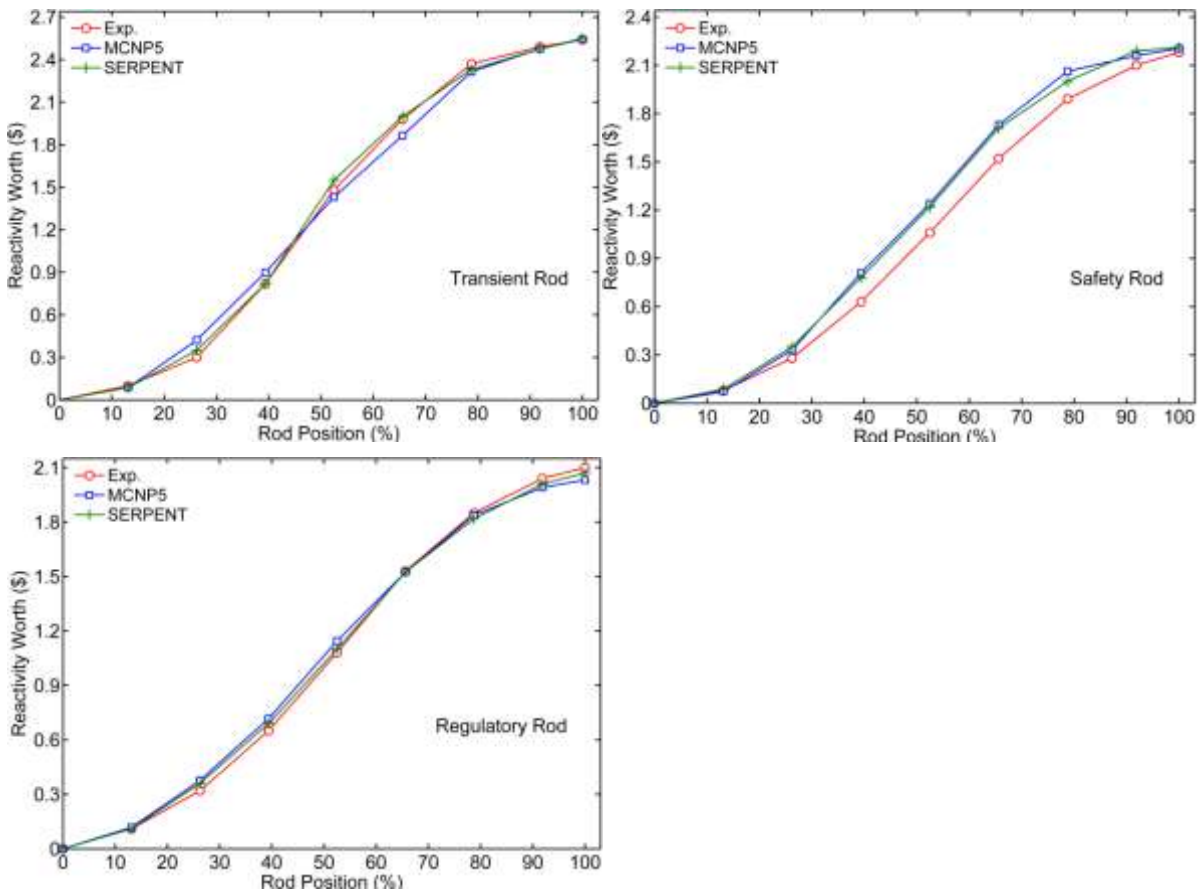


Fig 4. Reactivity worth of control rods as a function of rod position

4. Discussion and Conclusion

Although both MCNP5 and SERPENT codes are Monte Carlo-based computer programs, the cell definitions and the methods used for neutron transport calculation are different. Due to this reason, some differences appear inevitably even though all the reactor core parameters are completely modelled.

In case of the deterministic codes, the selected computational method is more dominant factor on the results, as shown in the Table 1. Furthermore, a 2-D geometry modelling needs more attention than a 3-D modelling since the geometric buckling and geometric simplifications become a major issue when the leakage of the reactor is quantified.

On the one hand, since thermal scattering cross-section libraries are not available for TRIGLAV and DRAGON codes, these codes leads to some under/over-estimation as seen in the related table and figure. In addition, deterministic codes are, at least for some cases, not well qualified to solve neutron diffusion/transport equation near highly thermalized areas.

From the point of computing time, the deterministic codes always give the results in short time typically less than one minute without depending on the computer requirements; but, containing higher relative true error. Conversely, stochastic codes generally yield more reliable results; but, require more running time for an acceptable computational error. They also require more memory and fast computers compared to the deterministic codes. All in all, it seems that the all the codes can be used to predict criticality analyses with sufficient accuracy.

Some analyses such as rod worth calculation cannot be done easily by the studied deterministic codes due to incapability of the codes in modelling of the complicated geometries. Such a kind of situations limits the user when a complicated system is modelled.

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ISOMER/GROUND BRANCHING TREATMENT IN COUPLED MCNP/ORIGEN2 BURNUP SYSTEM

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ABSTRACT

For conversion studies of its very compact core FRM II uses since 2009 as an alternative the coupled MCNP/ORIGEN-system, MonteBurns (MB). Comparison to results of the core design sequence Mf2dAb of the late '80s revealed some discrepancies as a lack of reactivity loss showed up. It was found, that this is mainly due to some missing fission products for the coupled MB-System in our case and that the resulting lack is only important for high flux reactors. The main single contribution to this deficiency was found for the isomer Pm148^m. For this case, both isotope states, ground and isomer must be included, but Pm148^m is not incorporated in the coupled MB-System although fully treated in ORIGEN2.

This work will show the way to overcome this deficiency with MB and reveal some details of treatment of pair ratios between ground and isomer states in ORIGEN. It was found, that ORIGEN corrects the pair ratios with settled values from its basic data library sets. Regarding a collected pool of experimental data, it is judged, that the correction should be improved for Pm-148. For all other pairs the effect of different n-capture ratios for the reactor calculations, particularly for reactivity values, is fully negligible.

1 Introduction

Through exploded computer power MonteCarlo (MC) methods for individual particle transport are exploited more and more, even for usually longer running burn-up calculations of 3d modelled reactor cores. For conversion studies of its very compact core FRM II uses since 2009 the coupled MCNP/ORIGEN-system, MonteBurns (MB). Comparison to results of the core design sequence Mf2dAb of the late '80s [Roe80] revealed some discrepancies as a lack of reactivity loss ($\Delta k_{\text{eff}}^{\text{MB_Mf2dAb}} = 0.0073 \pm 0.0003$) showed up [Frm10].

It was found, that this is mainly due to some missing fission products for the coupled MB-System in our case and that the resulting lack is only important for high flux reactors. The main single contribution to this deficiency results from the isomer Pm148^m. For this case, both isotope states, ground and isomer must be included for FRM II burn up, but Pm148^m is not incorporated in the coupled MB2.2-System although fully treated in ORIGEN2. It will be shown a way to overcome this deficiency with MB and reveal some details of treatment of pair ratios between ground and isomer states in ORIGEN.

2 ORIGEN burn up

ORIGEN is a computer code system for calculating the build up, decay, and processing of radioactive materials. The second major version ORIGEN-2 (in 2010, 2.2) is used meanwhile since more than 30 years in, without doubt, thousands of applications worldwide. It is based on data libraries that respect reactor differences in neutron spectra in principle. At FRM II we use it together with very extensive Monte Carlo neutronic calculations in most real core geometries for conversion studies.

Amongst the huge zoo of fission products there are several of isomer type, too. Although ORIGEN itself processes isomer and ground states in the coupled MCNP-ORIGEN scheme the parallel coupling of isomer and ground states in MonteBurns2.2 is not foreseen and needs extra programming. This was accomplished here and the changes in results are shown for the calculation of our reactor core as well as on a more general ground. In fact there is only one 'isomer/ground' nuclide pair, relevant for reactivity of high flux reactors, the one of Pm-148.

It was also found, that the n-capture pair ratios between ground and isomer states are treated in ORIGEN2 dependant on the chosen library. It is found, that the ORIGEN code corrects the pair ratios with the settled values from the basic libraries PWRU, BWRU and of other libraries with thermal and fast spectrum character, but that there are inconsistencies.

3 Coupled MCNP/ORIGEN burn up calculations for FRM II

Before 2009 only deterministic burn up procedures were used for the principal conversion studies [Frm05/Frm06][#]. A request from ILL in 2009 for exchange with results and methodologies in core studies promptly lead to realisation of the old idea for use of a coupled MCNP/ORIGEN-System as an alternative burn up method for FRM II [Frm10]. The main foundation for this, a fine 3d-model of the very compact core in its complicated surrounding, was already fully elaborated. Very quickly the MCNP-ORIGEN2.2 coupled version of MonteBurns2 of LAN Laboratory [MB2.2] could be installed and studied. Especially for core conversion studies this system showed up to be a very powerful tool without complicated work for data preparation beforehand.

3.1 Burn up model and adaptations

With regard to the former system Mf2dAb, the MB system is now nearly different from the scratch, so that a comparison of results covers also a wide variety in used data, model and methodology of calculation. For best comparison of the two methods and to reveal differences with best estimate one should stay as close as possible at the same model parameters.

The discrete elements of both burn-up procedures are very comparable. The core was partitioned into 7*10 radial/axial burn-up zones, now for MB into 8*6 zones. Since MB-2.2 could handle not more than 40 zones in the delivered version some changes had to be performed in both the perl-script <monteburns.pl> and the fortran code <monteb.f>. The same time stepping model* could be used as in the classical approach with about 10 steps over the whole cycle.

[#] TUM developed this very detailed module sequence Mf2dAb to cover all neutron physics aspects of the full fuel cycle of the reactor concept in 2d-cylindrical symmetry (r,z). It led finally to the core design of FRM II [3,4] with a single fuel element.

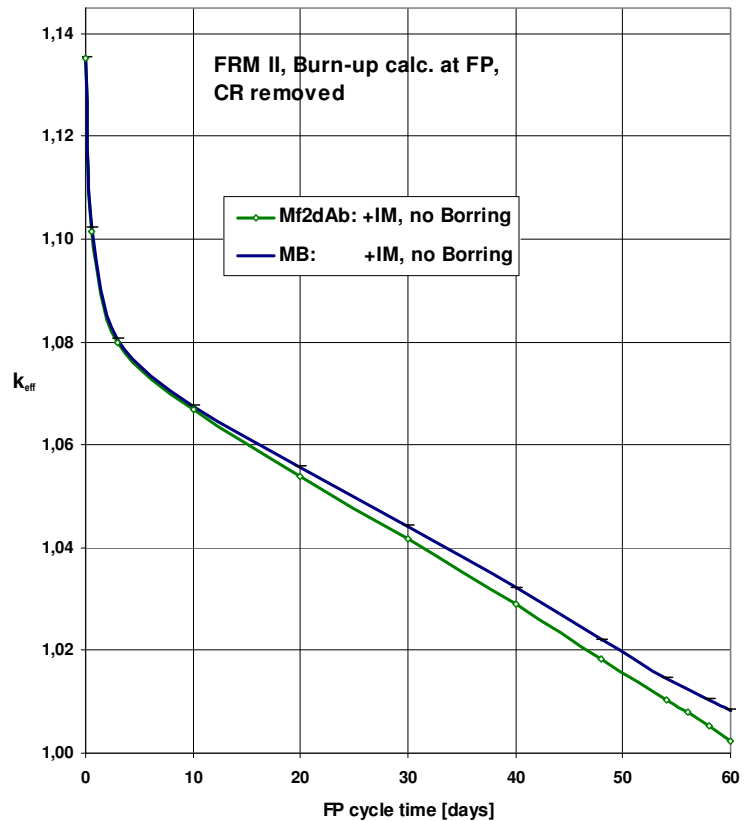
* A sound particularity of MonteBurns is that it evaluates for the mid of the time step and can use the flux estimations from this calculation for the intermediate state and even repeat the prediction step as often as guessed.

4 Results for core burn up in comparison

4.1 Reactivity loss

The reactivity of the core of FRM II over a full cycle is not only influenced by the core burn-up itself. Therefore no other burn-up than for the fuel was calculated for the comparison here. Other burnable/poisonable materials, from which the main ones are the inner reflector of material beryllium and the boron ring on bottom of the core, were not treated burnable. And because of the basic stochastic principal of the MCNP code a 'search mode for CR positioning' would add an extra degree of deviations and is not recommended for a principle system study. Thus the CR position stood in its end position for both calculation runs Mf2dAb and MonteBurns. Thereby a small systematic difference between both methods was derived for the reactivity loss over the cycle, a gap of $\Delta k_{\text{eff}}^{\text{MB_Mf2dAb}} = 0.0073 \pm 0.0003$ finally and nearly linear increasing with cycle time.

Fig. 1: calculated reactivity curve total different burn-up procedures Mf2dAb and MB (MonteBurns) over a full cycle of 60 days at full power (FPDs) for FRM II in theory without any CR movement (moderator inside, mode '+IM'). The last curve is then for the MB calculation with boron ring, that must be ignored for this comparison.



A closer discussion showed that the MB procedure used in its standard package taken from [MB2.2] lacks some important fission product isotopes in the case of FRM II. Besides several others with tiny or small importance one major isotope was revealed missing:

Pm-148m ($T_{1/2} = 41.3\text{d}$)

4.2 Missing isomer Pm-148m

With the modular system Mf2dAb it is easy to switch off specific parts and study at once differences as here with/without one fission product. It was found that Pm-148m accounts for $\Delta k_{\text{eff}}^{\text{Pm8m}} = 0.0030$ at the cycle end (EOC) through direct absorption and also build up of other absorbers as there is Sm-149.

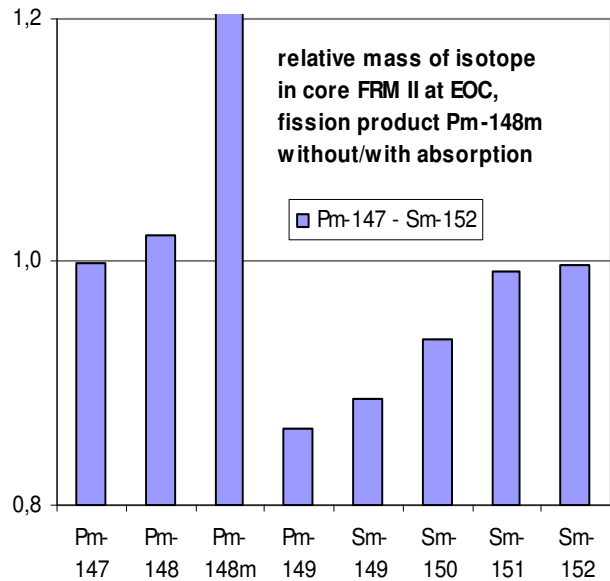
Fig. 2:

The nuclide chart excerpt [NC_K] reveals same major properties of the nuclide range around Pm-148, a nuclide for which both the ground as well as the isomer state can count as fuel poison.

Sm 147 14.99 1.06 · 10 ¹¹ a α 2.235; σ 56 σ _n , α 0.0006	Sm 148 11.24 7 · 10 ¹⁵ a α 1.96 σ 2.4	Sm 149 13.82 α 40100 σ _n , α 0.031	Sm 150 7.38 σ 102
Pm 146 5.53 a ε; β ⁻ 0.8... γ 454; 747; 735... σ 8400	Pm 147 2.62 a β ⁻ 0.2... γ (121...) σ 84 + 95	Pm 148 41.3 d; 5.37 d β ⁻ 0.4; β ⁻ 2.5 1.0...; γ 550; 1465; h (75...); 915... σ 10500; σ ⁻ 1000	Pm 149 53.1 h β ⁻ 1.1... γ 285... σ 1400
Nd 145 8.3 σ 47 σ _n , α 0.000012	Nd 146 17.2 σ 1.5	Nd 147 10.98 d β ⁻ 0.8; 0.9... γ 91; 531... e ⁻ σ 440	Nd 148 5.7 σ 2.4

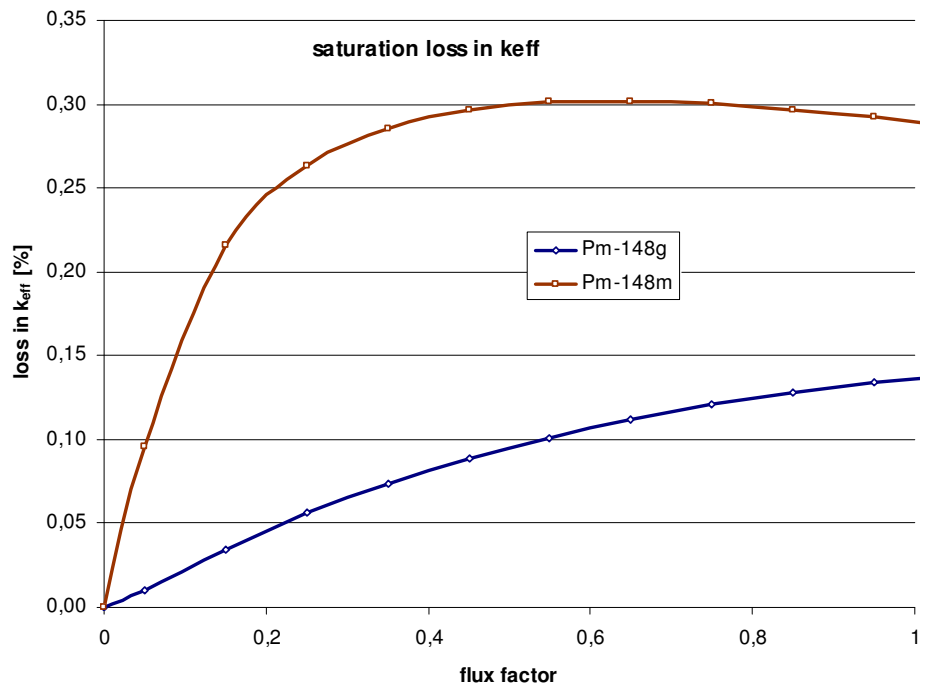
In Fig.3 it is depicted the disturbance of the isotope amount of the isotope range around the isomer Pm-148 when not providing the absorption cross section for Pm-148m. This causes a lack for the activation rates of the very strong absorbing isotopes Pm-149 and its daughter Sm-149 (also Sm-150) although included in the MB standard burn-up library in contrast to the isotope Pm-148m.

Fig. 3:
relative mass of isotopes in core FRM II at EOC, calculated with very flexible module sequence Mf2dAb without and with absorption of fission product isomer Pm-148m for a reactor cycle at full power (FP) of FRM II. The Pm-148m amount calculates 4.5 times higher without absorption of the isotope (MB standard case) and at the same time some parts of absorbing Pm-149 and Sm-149 and even Sm-150 amounts are missing. The amount of Pm-148g is calculated a view % too high, since more Pm-148m decays now to the ground state.



Or with other words, by providing Pm-148m in the coupled MCNP/ORIGEN system the whole neutron activation chain from Pm-149 to Sm-152 becomes much more populated here because of the high flux in the core. It was first stated in [Frm10] that this product (as for Xe-133 and Pr-143) is essential only in reactors with a high flux in the core and at the same time with cycle duration of month(s) instead typical NPP duration of years. While this is completely true for the two other isotopes, with Pm-148m there can also remain small degradation in reactivity for NPPs after a power run of some year of the fuel elements in lower flux conditions. This is studied analytically for an example of a water reactor with typical cross section data taken from the ORIGEN library PWRU*.

Fig. 4:
principle loss on k_{eff} for water reactors at EOC resulting from absorption on Pm-148 isotopes 'ground and isomer' at cycle end (FRM II) or at fuel reload (in a power reactor). A flux factor of 'One' would be typical for FRM II (running 60 days) and of about 1/10 for a power water reactor when having achieved about 600 days of operation.



* Although the PWRU value is somewhat too high for FRM II, this doesn't matter very much here.

The flux level in the fuel of the reactor was taken as a free parameter in this analytical study. A flux factor of 'One' would mean a reactor like the FRM II, reaching 60 full power days at cycle end. A typical power water reactor could have about 1/10 of the flux in the fuel and reach at least about 10 times the operation timespan in fuel average, so that the fuel burn before reactor reload can be regarded comparable in this somewhat simplifying study. But all relevant aspects can be taken from the diagram with pure analytical data:

- At FRM II the disturbance with the Pm-148m chain is about 0.29% in k_{eff} at the cycle (compare 0.30% given numerically by Mf2dAb), what is a lot for the single fission product isotope, when not regarded by the system*. The β -decay (41 days) path to Sm-148 is nearly dried out, more than 90% of the isomer go the Pm-149 absorption chain because of the high flux. The disturbance with the Pm-148g chain is nearly half the value with about 0,14% in k_{eff} at the cycle end. Although more Pm-148g is produced, the main path even with the high flux is still the β -decay (5.2 days) to merely absorbing Sm-148.
- Would FRM II operate double the time at the half power respectively flux levels, then Pm-148m would disturb maximal, because it is then produced slightly more at cycle end, as the fission product predecessor Nm-147 needs 16days in average to decay to Pm-147 and this delay weights more for a shorter operation time. The disturbance by the ground state would be lower, since Pm-148g vanishes then more by β -decay instead of transmutation by σ_a for neutrons.
- Then for a power reactor at a flux level of about 1/10 another effect rules out the behaviour. More and more Pm-147 β -decays (2.6 y) to low absorbing Sm-147 instead of being absorbed and transmuted to Pm-148 (m or g). Although 10 times longer operation time assumed, Pm-148g is rather negligible now for reactivity, since it also decays mainly by β -decay; nevertheless the remaining Pm-148m is still transmitted mainly to Pm-149 and should be fully regarded for reactivity studies at high and medium flux levels in the fuel.
- A simple respectation of Pm-148, either ground or isomer, in a usual term $\Delta k_{\text{eff}}^{\text{FissProd}}$, linear with fluence, is impossible for this complicated chains.

and (s. also later)

- The value for the production ratio Pm148m/ Pm148g is very relevant for the calculated reactivity disturbance over the whole range of the flux factor (except really low flux)

* When missing only as cross section in the transport code of the coupled system, then ORIGEN can use its library cross section for build up of the Pm-149 chain. The lack in k_{eff} is then about half of the value above, not very dependant on the used library Pm-148m cross section. This is the standard behavior of MB2.2 when installed.

4.3 Corrections in MB

For clearly better description of the reactivity loss over a full cycle of our reactor the standard burn-up library of MonteBurns needs an adjustment for FRM II to compensate about 10 missing absorber fission products. For most of them it is sufficient to look for a preprocessed cross section file for the isotope in MCNP and add the nuclide identifier simply to the list of relevant isotopes for MB.

4.3.1 Correction in MB for Pm-148m inclusion

In other cases as with Pm-148, where an isomer in parallel must be respected, the job is more complicated and it is not foreseen in MB. Nevertheless this is solved for our local version by some programming steps.

E.g. the MCNP code takes 61148.xx for the cross section of Pm-148g. When coupled for ORIGEN, there is simply added '0' or '1' for nuclide identification, e.g. '611480' for the ground and '611481' for the isomer of Pm-148. One can provide now a cross section for Pm-148m with an identifier '61142', a number that is always kept free and which can be easily added for use in MCNP. MB treats this number as usual as '61148' for Pm-148g and will produce also cross section tally output files with those identifiers for input into ORIGEN. It is now sufficient to change the identifier in this tally files from '611420' to '611481', done inside the perl-script <monte-burns.pl>#, and ORIGEN will process it correctly and give new nuclide densities as output. This output needs now the vice versa correction in the same perl-script, so that MB will further provide the correct densities for automatic use in MCNP. The coupled cycle MCNP→ORIGEN→MCNP is thus elaborated fully for the isomer/ground pair Pm-148 and the same could be done for any other pair, although not regarded necessary here.

4.3.2 Correction in MB for correct production ratio of pair Pm-148m/g

When closer studying the results with the fully incorporated Pm-148m chain, some strange behaviour was found for the produced nuclide ratios between Pm-148m and Pm-148g.

MB is as versatile as possible with its spectral treatment of neutron cross sections. It can take the best available data files that are used also in MCNP and condense them in a quite appropriate manner for use in the burn up in ORIGEN, thus widely eliminating the use of predefined cross section data in the ORIGEN libraries. Nevertheless some data need to be known besides as there is the ratio for parallel production of isomer and ground states in this case. Those are provided now by ORIGEN, better speaking through its libraries. It was found that any ORIGEN library gives one predefined value for this ratio for any possible pair and that this value is used in MB, but it can differ clearly from library to library.

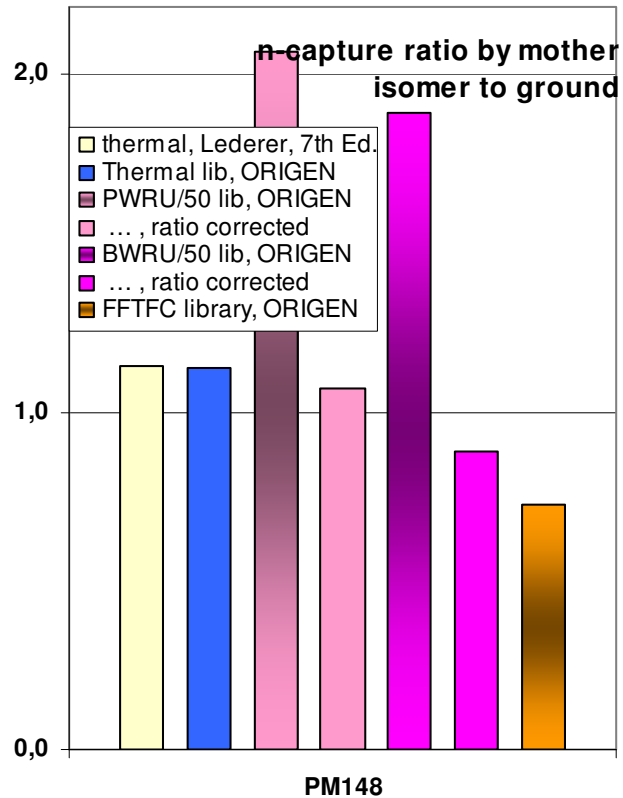
On the other side shows a study in literature [BNL73, CompRI, Fenn67, Sman62, ...] no remarkable spectral deviation of this ratio. The most common value when absorbing a neutron in Pm-147 is a ratio of Pm-148g/Pm-149m of slightly above One, e.g. 52% to 48% or $\text{rat}_{148_{\text{mg}}}=1.1$ for both thermal and epithermal or resonance energy range. But instead the production ratio in the output is clearly closer on the Pm-148m side when staying at the PWRU library in MB in our case. It is about $\text{rat}_{148_{\text{mg}}}^{\text{PWRU}}=2.1$ and one could at once suspect a simple arithmetic miss-interpretation between producer of library and the author of the MB procedures. Being curious one can find a comparable value far above One for the BWRU library of $\text{rat}_{148_{\text{mg}}}^{\text{BWRU}}=1.9$. ORIGEN has also a THERMAL library that ignores other than thermal neutrons and now one can find exactly the literature value of $\text{rat}_{148_{\text{mg}}}^{\text{TH}}=1.1$.

Going even more into depth one can pick out the exact values of [Sman62] settled into THERMAL library. That means that both authors had the same interpretation here, meaning that the first

It will be sufficient to do it in the script directly after the text "Run origen for complete outer step", but better do it also for the predictor steps.

value in the cross section files is pure σ_a^g and the one for the isomer column is σ_a^m . The values in the power water reactor libraries (PWRU, PWRU50, BWRU, BWRUx ...) indicate rather clearly, that the first value is settled there with the interpretation of σ_a^{g+m} . The condensed values σ_a^{g+m} of MB for Pm147 confirm this argument for the undermoderated core of FRM II, giving values comparable to those settled down in PWRU and BWRU. But MB needs there pure σ_a^g and this leads finally to the invalid factors $\text{rat148}_{\text{mg}}^{\text{PWRU}} \dots$ calculated and used by MB out of the ORIGEN libraries. The story seems to be the same for other ground/isomer pairs, e.g. for Eu-152, but they are usually totally negligible for reactor performance.

Fig. 5: production ratios for the Pm-148m/g pair from literature and from MB system results on base of different ORIGEN libraries. There seems to exist a misinterpretation in the system, where it is put σ_a^{g+m} into the light water libraries but MB interprets it always as pure σ_a^g . For the THERMAL library the value σ_a^g is settled and thus interpreted correctly, but this library is not adequate for FRM II because of other reasons. One can instead correct for this misunderstanding and receive the expected ratio. There seems to be a trend in the ORIGEN libraries, the harder the spectrum from TH, over PWRU, BWR (both corrected, too) to the fast lib FFTFC (not corrected here), the lower the ratio is settled down.



Based on the literature study the author of this article proposes to use the literature value $\text{rat148}_{\text{mg}}=1.1$, a value that is also settled down in the library used by the deterministic system Mf2dAb, instead of values far away from it for any water moderated reactor. The use of the THERMAL lib is not adequate for FRM II because of other reasons, thus it has a clear consequence when calculating the burn up with MB on base of the power water libraries and without correction for the literature value. This correction can be adapted to MB in the fortran code <mon-teb.f> in routine 'worxs' for the variable 'ratio' when the nuclide identifier is '611470'.

Without correction MB gives a ratio rat148_m around 2 and:

- clearly too much Pm-148g and is produced and too less Pm-148m and Pm-149 chain follower nuclides;
- the reactivity under full power is thus given somewhat too high, with $\Delta k_{\text{eff}} = +0.05\%$ against calculated with the correct ratio $\text{rat148}_{\text{mg}}=1.1$. This value can be also derived from the diagram of figure 4. So the effect on the reactivity by $\text{rat148}_{\text{mg}}$ is rather small and it needs a fine 'magnifying glass' to catch this detail.
- And it has also an influence on the poisoning of the reactor with Sm-149 after shutdown.

SUMMARY / OUTLOOK

Comparison of burn up results of two different systems used for conversion studies of FRM II research reactor revealed some discrepancies. It was found, that a lack of reactivity loss is mainly due to some missing fission products for the coupled MCNP/ORIGEN-system, MonteBurns'. The main single contribution to this deficiency was found for the isomer Pm148^m. For this case, both isotope states, ground and isomer must be included. It was shown that, while Pm148^m is incorporated only partly in the coupled MB-System, it can be fully integrated there.

The treatment of pair ratios between ground and isomer states in ORIGEN is another aspect thereby. It was found, that ORIGEN corrects the pair ratios with settled values from its basic data library sets. Regarding a collected pool of experimental data, it is judged, that the values are settled not conform in the different libraries and that the value is taken by MB with a miss interpretation for power water libraries. Thus a relevant correction for burn up with Pm-148 is needed.

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