





Dati nucleari per la sicurezza reattore: Analysis of the ZED-2 reactor for the benchmarking of the newly measured Gadolinium capture cross-sections

P. Console Camprini, F. Rocchi, A. Guglielmelli, D. M. Castelluccio, A. Mengoni, M. Frisoni

Report RdS/PAR2018/119

# DATI NUCLEARI PER LA SICUREZZA REATTORE: ANALYSIS OF THE ZED-2 REACTOR FOR THE BENCHMARKING OF THE NEWLY MEASURED GADOLINIUM CAPTURE CROSS-SECTIONS

P. Console Camprini, F. Rocchi, A. Guglielmelli, D. M. Castelluccio, A. Mengoni, M. Frisoni (ENEA)

Dicembre 2018

Report Ricerca di Sistema Elettrico

Accordo di Programma Ministero dello Sviluppo Economico - ENEA Piano Annuale di Realizzazione 2018 Area: Generazione di Energia Elettrica con Basse Emissioni di Carbonio Progetto: Sviluppo competenze scientifiche nel campo della sicurezza nucleare e collaborazione ai programmi internazionali per il nucleare di IV Generazione. Linea: Sviluppo competenze scientifiche nel campo della sicurezza nucleare Obiettivo: Dati nucleari per la sicurezza reattore Responsabile del Progetto: Federico Rocchi, ENEA

		Sigla di identificazione	Distrib.	Pag.	di		
ENER Ricerca Siste	ma Elettrico	ADPFISS-LP1-129	L	1	18		
Analysis of the ZED-2 reactor for the benchmarking of newly measured Gadolinium capture cross-sections							
Descrittori		4 E					
Tipologia del documento:	Rapporto Tecnico			e.			
Collocazione contrattuale:	: Accordo di Programma ENEA-MSE su sicurezza nucleare e						
	reattori di IV genera	azione					
Argomenti trattati: Neutronica							
Reattori Nucleari Evolutivi							
8 - P	Dati Nucleari						
4	Calcoli Monte Carlo						
Sommario							

In nuclear technology, a detailed knowledge of nuclear data is of primary importance to optimize the design characteristics of nuclear facilities and to enhance related safety margins. In particular, Gen-III and Gen-III nuclear power reactors take advantage of neutron absorbing materials - called burnable poisons - that are mixed with the fuel in the pins of certain Fuel Assemblies (FA) in the core and are consumed during the cycle. This is a common practice that allows to pack more fissile material into each FA at the beginning of the cycle. This increases the amount of energy extracted from it over the whole cycle with no safety issues, since the poison compensates the extra-reactivity. There is a consequent economic gain for the utility in the availability factor and plant capability. The most important burnable poison is gadolinium, through its odd isotopes <sup>157</sup>Gd and <sup>155</sup>Gd which have a high capture cross-section. An improvement of the current nuclear data for these gadolinium isotopes has a feedback on nuclear plant management and safety. For that reason, a joint ENEA and INFN research team has carried out new measurements for these nuclides at the n TOF facility at CERN. In the present report, the new evaluated nuclear data are considered in comparison to standard ENDF/B-VII.1. The ZED-2 nuclear research reactor (at Chalk River Laboratory - CRL, Canada) is considered as a possible case study for such evaluation, since a reference experiment with gadolinium diluted in the moderator has been performed there. Some simulations have been made with different quantities of gadolinium poison in the reactor moderator, employing the MCNP6.1 Monte Carlo transport code. The neutron spectrum in the moderator is calculated as well as k effective and its sensitivity to the microscopic neutron capture cross-section of <sup>157</sup>Gd and <sup>155</sup>Gd. The results highlight the relevance of the system since it presents a thermal neutron spectrum and it is sensitive to the data of interest. Comparison with results obtained at the ZED-2 facility by the CRL research team is not straightforward due to employment of different nuclear data sets and simulation parameters. It is shown that model calibration cannot cover and compensate all these aspects. More details are required and a sensitivity calculation concerning other parameters (temperature of fuel, moderator and thermal scattering data) is needed. Possible other benchmark cases should be investigated as well.

#### Note

#### Autori:

P. Console Camprini, F. Rocchi, A. Guglielmelli, D.M. Castelluccio, A. Mengoni, M. Frisoni

Copia n.	2 1	4	In carico	) a:		
2			NOME			
-			FIRMA			
1			NOME			
	e1 		FIRMA			
0 EMISSIONE	20.01.2010	NOME	P. Console Camprini	K. W. Burn	F. Rocchi	
	28-01-2019	FIRMA	Bhililyu	KAZ	Sedenco Docit	
REV.	DESCRIZIONE	DATA		REDAZIONE	CONVALIDA	APPROVAZIONE



# Table of Content

1.	Inti	roduction3				
2.	ZEC	D-2 Nuclear Research Reactor5				
3.	Description of the Test at ZED-2					
4.	Ser	nsitivity analysis for ZED-28				
5.	Un	certainty of the Monte Carlo model and Calibration11				
5	.1	Model Calibration at CRL12				
5	.2	Model calibration at ENEA13				
6.	Res	sults and Comparisons 14				
7.	Cor	nclusions				
8.	Acł	knowledgments				
9.	Ref	ferences				



#### 1. Introduction

Within the framework of the continuous improvement of nuclear data supporting nuclear reactor design, a number of experimental activities have been carried out in order to produce neutron cross-sections with enhanced precision and reduced uncertainty.

In nuclear reactors, some materials have particular characteristics that are important to assure that the fission chain reaction can be sustained efficiently and in a stationary fashion. The objective is to establish a neutron population and keep it constant with an energy distribution which is relevant for fission of <sup>235</sup>U, <sup>239</sup>Pu or other fissile nuclides. In order to achieve this task, materials with different properties are considered at the design phase: the fuel material contains the nuclides undergoing fission, the moderator is important to slow down fast neutrons generated through fission and the coolant is necessary to transfer the heat produced out of the system keeping all the temperatures constant.

Absorbers are materials which exhibit a significant capability of capturing neutrons, with the neutron absorption cross-section being particularly high at the average energy of the system. Nuclear power plants are provided with specific absorbing devices, called control rods, to be able to modify the intensity of the neutron flux and then to increase or to reduce the total fission reaction rate inside the core and thus the output thermal power.

Moreover, absorbing nuclides are also utilized in Gen-II and Gen-III nuclear power reactors (such as PWRs and BWRs) as burnable poisons which are mixed with the fuel materials inside the fuel pins. This is a common practice in the nuclear industry and enables the extension of the in-core residence time of a Fuel Assembly (FA), improving the duration of a core cycle. In fact, a longer duration of the period between core loadings requires a higher fissile content at Beginning of Life (BOL) to guarantee that the multiplication factor of a certain FA – and of the whole core as well – remains above unity to maintain the system critical up to End of Life (EOL). Conversely, increasing the amount of fissile material in the core at BOL normally produces an excess in reactivity that can require additional safety devices. This issue is particularly relevant for start-up cores as well as for equilibrium cores.

For that reason, burnable poisons are added to the fuel as dopants which can compensate the initial excess reactivity with concurrent absorption reactions – lowering the integral multiplication coefficient of the system.

Fuel pins are doped with gadolinium and inserted in the FA's. The gadolinium is consumed by the neutron flux simultaneously with the burnup of the fuel through fission. The combined effect of the two processes limits the variation of k effective over the cycle – in practice in the first part of the cycle k effective increases as the gadolinium is burnt, then after reaching a peak k effective decreases in the latter part of the cycle.

Gadolinium oxides are used and mixed with the ceramic matrix of both  $UO_x$  and MOX fuels obtaining sintered composite materials. The most common chemical form is gadolinium oxide  $Gd_2O_3$  in which the gadolinium isotopic mix is the same as the natural abundance. The isotopes providing an absorbing effect are the odd isotopes such as <sup>157</sup>Gd and to a lesser extent <sup>155</sup>Gd.

A detailed knowledge of the nuclear data concerning the gadolinium odd isotopes is therefore very important for all the relevant aspects of nuclear reactor management. Foremost, the extension of the in-core period can enhance the load factor and the plant availability reducing the ratio between the refuel time and the operational time. Extension of the fuel cycle means an economic gain for the nuclear energy utility reducing the payback time of the plant and the specific cost per unit energy produced.

An improved evaluation of the gadolinium capture cross-section data implies both an enhanced definition of the residual reactivity penalty at FA discharge and a more precise characterization of the reactivity peak during the FA life. This is a crucial aspect in the determination of the multiplication factor at the discharge and is very important for the criticality safety studies at the spent fuel pools. The latter are zones of the plant in which spent FAs are stored in a cooling environment and for this reason require particular studies in order to guarantee that criticality conditions are never reached.



For the sake of completeness, it is worth saying that gadolinium is also a fission product, that is also produced in small amounts among the fission fragments. Improved nuclear data can also, as a by-product, provide a better insight into the core composition during in-core irradiation.

CANDU reactor technology may also take advantage of better measurements of gadolinium cross-sections since gadolinium oxide is diluted in the heavy water moderator in the case of an accident so as to shut down the system.

All these technological motivations make gadolinium a very important element in nuclear reactor design. Therefore, an improvement of the currently utilized cross-sections looks to be an activity of relevance to the nuclear industry [1]. The uncertainty associated with the gadolinium neutron capture cross-section in the relevant thermal energy region has been considered in sensitivity analyses for many criticality benchmarks [2].

Monte Carlo and deterministic simulations carried out on a large number of criticality benchmarks have highlighted how much these uncertainties impact the multiplication factor and have confirmed the strong interest in improving the precision of these data [3].

Thus, ENEA and INFN (the Italian National Institute for Nuclear Physics) researchers have performed last year some experimental tests at the n\_TOF (neutrons Time Of Flight) facility located at CERN (European Center for Nuclear Research) in order to obtain a new neutron capture cross-section data set for gadolinium odd isotopes <sup>157</sup>Gd and <sup>155</sup>Gd. The measurements were able to provide improved data, reducing the uncertainty from about 6% in the high sensitive thermal region to about 2-3% [4,5].

After the measurements were completed and the data processed, in a successive step it was necessary to perform a set of relevant simulations to verify the impact of the new cross-sections on the main relevant criticality benchmarks for these nuclides. Criticality calculations performed with a standard nuclear data library are thus compared with calculations in which only particular nuclides are substituted in order to evaluate the impact on the multiplication factor due to the specific data.

In this report a part of this second step is described. The ZED-2 research nuclear reactor, which is located at the Chalk River Laboratory (CRL, Canada), is considered. This facility is of particular interest since an experimental campaign has been carried out to measure the impact on the multiplication factor of the system (k effective coefficient) of gadolinium diluted in the moderator inside the reactor pool [6]

Starting from open publications and some input files provided to ENEA by IRSN and by the CRL Canadian research team, preliminary calculations have been performed to check whether the available data are sufficient to consider ZED-2 a good benchmark to assess the change in criticality due to the new neutron capture cross-sections for <sup>157</sup>Gd and <sup>155</sup>Gd measured by the ENEA and INFN team.

Simulations of ZED-2 performed by CRL and reported in the open literature involve a particular in-house nuclear data set called E70CRL [7] based on ENDF/B-VII.0, specifically prepared for the ZED-2 facility. These results and the methodology are considered and used as reference.

The average neutron spectrum inside the moderator is computed and the related sensitivity to the gadolinium data is obtained. In addition, the simulation procedure carried out by the Canadian research team is compared to the calculation scheme to be implemented in this work, starting from open nuclear data ENDF/B-VII.1 and standard room temperature parameters. Moreover, a calibration of the model is proposed according to the method described by the CRL team.

The final conclusions state how the currently available data and parameters are not sufficient, at present, to perform benchmark simulations. The CRL calculational results used here as reference were generated with nuclear data that were not available to us. Employing the available ENDF/B-VII.1 data meant that it was not possible to completely compensate for the difference in nuclear data with a different calibration coefficient in the simulations. As a consequence, it has not been possible to unambiguously establish a reference critical configuration against which the new ENEA/INFN <sup>157</sup>Gd (and <sup>155</sup>Gd) data may be tested. The calibration procedure in this experiment should probably be revisited. Furthermore, other gadolinium benchmarks should be considered.



## 2. ZED-2 Nuclear Research Reactor

In order to perform a numerical evaluation of the impact of the new measured capture cross-sections of gadolinium, the ZED-2 research nuclear reactor has been considered as a first possible reference benchmark. This reactor is located at the Chalk River Laboratory (CRL, Canada) and is of particular interest because an experimental campaign has been carried out there, to evaluated the absorption effect due to gadolinium oxide diluted in the moderator.

The Canadian nuclear safety agency required that particular test to assess the impact of gadolinium nuclear data adjusted by Leinweber [8] compared to the standard ENDF/B-VII.0 release.

ZED-2 is a tank-type research reactor (see Figure 1) which presents a calandria tank made up of an aluminum cylinder of about 3.4 m both in diameter and height. It is surrounded by a graphite reflector radially and below. It is filled inside by high purity (>98 wt%) heavy water that constitutes the moderator of the system. Criticality is reached through adjusting the moderator level. A certain number of fuel channels can be installed from the top to form the reactor core. The array of fuel assemblies which forms the core as well as the core pitch are arranged and modified from test to test, according to particular needs and neutronic parameters to be reproduced. Inside each fuel channel five fuel bundles of some 50 cm in length are accommodated.

The configuration of the reactor core for the present measurements is shown in Figure 2. The core is composed of 52 fuel channels: 48 channels are filled with Low Enriched Uranium (LEU) grade fuel and the remaining 4 channels consist of Recovered Uranium (RU) fuel bundles. The lattice is arranged in a square pattern with a 24.5 cm pitch. The channels are simply air-cooled since this is a zero-power test [6].



Figure 1) ZED-2 reactor vertical cross-section

Figure 2) ZED-2 core configuration

The reactor model used in the present study has been prepared by means of the Monte Carlo code MCNP6.1 [9], since this is considered a reference approach for detailed simulations. In fact, this method is able to deal with continuous energy nuclear data and can describe complex tridimensional geometry.

The reactor tank and some structural components around are modeled according to experimental measurements. Inside the reactor tank the core array is defined and all fuel bundles are reproduced according to both enrichment levels: LEU and RU.





Figure 3) ZED-2 reactor: MCNP6.1 model (vertical)



Figure 5) ZED-2 reactor: array pattern (south-west)



Figure 4) ZED-2 core: MCNP6.1 model (horiz.)



Figure 6) ZED-2 fuel bundle (pins and air inside)

Figure 3 to Figure 6 report some details of the Monte Carlo model utilized for the present study.

The main experimental parameters considered by the CRL team include the critical height, temperature and purity of the moderator, as well as the temperature of the fuel. Such information is relevant to know which parameters may impact the simulations. Further studies will look at the sensitivity of k effective to some of these parameters (for example in our simulations we used room temperature for both the fuel and moderator).



# **3.** Description of the Test at ZED-2

The aim of the experimental campaign carried out at the ZED-2 nuclear research reactor at CRL is to compare the neutron capture cross-sections for odd gadolinium isotopes <sup>157</sup>Gd and <sup>155</sup>Gd that are reported in standard ENDF/B-VII.0 and ENDF/B-VII.1 nuclear data libraries with new adjusted data obtained by the Leinweber research group. The idea is to provide a verification of the impact of the adjustments on the multiplication factor of a nuclear system. An experimental setup is prepared, then Monte Carlo simulations are performed.

First, the ZED-2 facility is run in a critical state with the core fueled according to the configuration described in the previous section: criticality is reached by adjusting the heavy-water moderator height in the reactor tank. This is the reference configuration for the following tests.

Then gadolinium is diluted in the moderator according to the naturally occurring abundance of gadolinium isotopes. The test is repeated with 3 different quantities of gadolinium dispersed in the moderator: 0.5 ppm in the first configuration, 1.0 ppm in the second test and 1.5 in the third experiment.

In each case the facility is maintained critical through regulation of the critical height of the moderator, measured with particular precision (see Table 1).

Case	Nominal Gd Conc. [ppm]	Moderator Purity [wt% D <sub>2</sub> O]	Channel Temperature [°C]	Moderator Temperature [°C]	Critical Height [cm]
Gadolinium G1	0.0	98.748	21.80	21.70	131.585
Gadolinium G2	0.5	98.748	21.75	21.79	138.248
Gadolinium G3	1.0	98.744	21.65	21.89	145.632
Gadolinium G4	1.5	98.739	21.45	22.51	153.926

Table 1) Gadolinium test series with different concentrations in moderator

Next a second set of experiments is carried out to provide a reference for the calibration of the model. Boron is diluted in the moderator instead of gadolinium. Since the absorption cross-section of this element should be known with a negligible uncertainty, it is considered as a reference.

A set of 3 different boron concentrations is considered: 2.0 ppm, 4.0 ppm and finally 6.0 ppm. The following Table 2 summarizes the boron experimental campaign.

Case	Nominal B Conc. [ppm]	Moderator Purity [wt% D <sub>2</sub> O]	Channel Temperature [°C]	Moderator Temperature [°C]	Critical Height [cm]
Boron B1	0.0	98.743	21.50	21.55	131.650
Boron B2	2.0	98.742	21.30	22.05	139.420
Boron B3	4.0	98.740	21.63	22.19	148.248
Boron B4	6.0	98.738	22.15	22.53	158.442

Table 2) Boron test series with different concentrations in moderator

Each configuration is kept critical and the stationary neutron population is measured. It is then verified that the experimental value of the multiplication factor is unity, within experimental uncertainty.

Through the concentrations of poisons and the values of the critical heights, the simulations can be prepared and the multiplication factor of each test can be computed with the Monte Carlo MCNP6.1 code.



## 4. Sensitivity analysis for ZED-2

Interest in ZED-2 to test the new gadolinium cross-sections has been first verified through preliminary simulations of the ZED-2 model, by means of MCNP6.1.

The multiplication factor has been computed for all gadolinium cases: G1, G2, G3 and G4 reported in Table 1. The calculations performed at ENEA have been made with the ENDF/B-VII.1 nuclear data set and related thermal scattering data  $S(\alpha,\beta)$ . Both data sets are evaluated at 20.42 °C (293.57 K). The heavy-water moderator purity, compositions of gadolinium and critical heights utilized are as in Table 1.

The first calculation dealt with the spectrum in the moderator. The most effective absorption for gadolinium is in the thermal range, thus a request for the system is to provide a neutron spectrum which is mainly thermal. Plots of the results are in Figure 7 and Figure 8. Normalized spectra are shown both per unit energy (Figure 7) and per unit lethargy (Figure 8), for all the gadolinium cases: G1, G2, G3 and G4. The error bars represent an uncertainty of one standard deviation that is for all cases well below 1%.

Results confirmed the interest in ZED-2 for the purpose of this study. The neutron system is mostly thermal with energy about 0.1 eV. The lethargy plot in Figure 8 illustrates the whole slowing down region down to the thermal peak with the classical behavior of a thermal system.

The gadolinium cases present an increasing amount of diluted poison from G2 to G4. The trend that turns out from the plots G1 to G4 in Figures 7 and 8 is consistent: there is a slight reduction in the thermal fraction since increased gadolinium provides higher thermal absorption and a consequent reduction in the thermal fraction: the spectrum tends to get harder.





Figure 7) Neutron spectrum in the moderator of ZED-2 reactor for G1, G2, G3 and G4 (per unit energy)

	Sigla di identificazione		Distrib.	Pag.	di
Centro Ricerche Bologna	ADPFISS-LP1-129	0	L	9	18

ZED-2 Reactor - Test Cases - Neutron Spectrum

0.4 0.35 Ħ ZED Spectrum per unit Lethargy [--] 0.3 0.25 Case G1: Spectrum Case G2: Spectrum Case G3: Spectrum Case G4: Spectrum 0.2 0.15 0.1 0.05 0 1.00 E-4 1.00 E-2 1.00 E+0 1.00 E+2 1.00 E+4 1.00 E+6 Energy [eV]

Figure 8) Neutron spectrum in the moderator of ZED-2 reactor for G1, G2, G3 and G4 (per unit lethargy)

Moreover, a sensitivity analysis has been carried out again with MCNP6.1. The sensitivity of the multiplication coefficient to the variation of the microscopic capture cross-section of both <sup>157</sup>Gd and <sup>155</sup>Gd is computed. Specifically, the quantity of interest is the fractional variation of the k effective of the system corresponding to the unitary fractional variation of the capture cross-section in question. It is a result which is provided according to a specified energy binning of the cross-section which is – for the sake of consistency – the same energy division as employed for the spectrum calculation.

Results are provided in Figures 9 and 10. Case G1 is the only one in which no gadolinium is present in the moderator. Notwithstanding, it is present in very small amounts inside the graphite reflector region. A sensitivity calculation has been performed anyway for the sake of completeness and to highlight the important impact that is found in the other G2, G3 and G4 cases.

Figure 10 highlights how the case G4 is the most sensitive to a small variation of the gadolinium capture cross-section - the amount of poison tends to amplify the sensitivity to the microscopic cross-section. We see in fact from Figure 10 and Table 1 that the sensitivity is quite closely proportional to the concentration of gadolinium in the moderator. If the gadolinium data is correct, errors in k effective reflect errors in the modelled gadolinium concentration.

In addition, the calculations confirm the different impact on the multiplication of the <sup>157</sup>Gd and the <sup>155</sup>Gd isotopes. As natural gadolinium is employed (for which the concentrations of <sup>157</sup>Gd and <sup>155</sup>Gd are similar), the results reflect the fact that <sup>157</sup>Gd has a higher absorption cross-section compared with <sup>155</sup>Gd.

ZED-2 is thus useful and interesting for the purpose of this evaluation. Thus we may proceed to verify whether the data and methodology employed by CRL can be extended to employment of ENDF/B-VII.1 and in particular whether uncertainties in other cross-sections in ENDF/B-VII.1 have a non-negligible impact on k effective.









ZED-2 Reactor - Test Cases 2,3,4 - Sensitivity

Figure 10) Sensitivity of k effective to capture cross-section of <sup>157</sup>Gd and <sup>155</sup>Gd: for cases G2, G3 and G4

### 5. Uncertainty of the Monte Carlo model and Calibration

The numerical model is prepared with MCNP6.1 and thus a calibration process is required to allow a comparison between experimental and calculational results. Once a numerical model is utilized, it involves a twofold source of uncertainties: the errors introduced according to the model definition (errors due to simplification) and the errors associated with parameters obtained experimentally that must be utilized but that are not exactly known (errors due to model data uncertainty).

In addition to the choices of the user concerning the design of the model, the simulations involve external input parameters that come with associated uncertainties: this is the case of nuclear data.

The following list reports the main sources of uncertainty in the simulations:

- 1) geometry description of the core model (in particular the fuel channel)
- 2) fuel enrichment and composition
- 3) critical height of the heavy-water moderator
- 4) purity of the heavy-water moderator
- 5) effective concentration of the poison diluted in the moderator
- 6) neutron capture cross-section of the diluted poison (gadolinium only, boron uncertainty is negligible)
- 7) cross-sections of all the other materials presently used in the simulation
- 8) stochastic error associated with the Monte Carlo simulation

The combination of all these sources of uncertainty yields an overall error associated with the final output of the simulation that is the multiplication factor of the system. The effect of all these uncertainties, taken together, yields an underestimation of the simulated value with respect to the experimental measurement of k effective of around 200-250 pcm (with a standard deviation of around 6 pcm) [6].

The calibration of the model is the attempt to find a factor of proportionality between experimental data and simulated values. This aims at correcting the systematic errors, of course, under the hypothesis that the adjusted parameter is linear with the reference output against which it is compared.

We underline here that when we have two sets of simulations, each with its own sources of uncertainty, we must distinguish between the parameters that are the same in each simulation and those that are not the same. In our particular case we have the gadolinium simulations and the boron simulations. Parameters that are the same are all cross-sections apart from boron/gadolinium, the fuel geometry, the reactor geometry, etc. Parameters that are different are the boron/gadolinium cross-sections and the concentrations in the moderator, in particular the concentrations adjacent to the fuel. If we neglect spectral effects, errors in parameters that are the same in each set of simulations generate the same errors in k effective.

In the case that an uncertainty exists in the boron neutron capture cross-section, cases B2, B3 and B4 will not provide the same result for k effective since the same error in the microscopic cross-section is amplified by a term that is the boron concentration in the moderator. Assuming instead that the boron capture cross-sections are available with negligible uncertainty – and no other uncertainties are present - it is possible to suppose that all cases with boron differ by the Monte Carlo statistical uncertainty, at most. Such a configuration with no significant – or negligible – sources of error has to be considered as a reference situation. The related model is then adjusted with respect to it in order to give consistent results for the simulation: this process is called calibration.

In this case, the calibration of the model is obtained by adjusting the poison concentration diluted in the moderator. That means that all the global uncertainty associated with the model – in the reference case - is assumed to be proportional to that poison concentration. The uncertainty of poison concentration is not easy to evaluate since, although the amount of poison is well known, the effective amount of moderator volume to be considered for the concentration calculation is not easy to compute: the fluid in the tank is static and it is difficult to obtain a stationary situation of an optimal dilution.



In practice, k effective is evaluated in the case without boron in the moderator: case B1. Then, the simulation is performed for case B4 in which a nominal concentration of 6.0 ppm boron in considered. The boron concentration in case B4 is corrected by some factor, in order to obtain k effective of case B4 equal to case B1 – within an interval that is equal to the Monte Carlo statistical uncertainty.

The correction coefficient is then applied to all other cases in the boron series. The idea is to use such a coefficient to correct all nominal concentrations of poison in the moderator.

After the calibration, it is important to consider if this process can cover and involve sources of error according to a linear approach. In the case of the CRL simulations, the calibration served to correct the amount of poison dissolved in the moderator as well as to understand the other errors and uncertainties in the model [6]. An important question to be investigated is that with open data ENDF/B-VII.1 (different from those used by the CRL team) and related temperatures at cold conditions (standard room temperature), whether calibration can attain a sufficient degree of precision. The calibration procedures used by both the CRL research group and the ENEA team are illustrated in the following paragraphs.

#### 5.1 Model Calibration at CRL

The research team at CRL computed the calibration and it turned out that such a correction for the boron concentration in the moderator is about -1.2% with respect to the nominal values. This coefficient was verified by applying it also to cases B2 and B3 resulting in a very satisfactory near-horizontal distribution (i.e. near-constant k effective). They propose the adjusted concentrations for the simulations reported in Table 3 (with the critical height unaltered from the experiment). The calculations at CRL are carried out with MCNP5-1.60 and the E70CRL nuclear data set, which is based on ENDF/B-VII.0.

Case	Adjusted B Conc. [ppm]	Critical Height [cm]	Multiplication Coefficient (keff)
Boron B1	0.0	131.650	0.99785 ± 0.00006
Boron B2	1.976	139.420	0.99788 ± 0.00006
Boron B3	3.952	148.248	0.99800 ± 0.00006
Boron B4	5.928	158.442	0.99779 ± 0.00006

Table 3) Boron adjusted values and k effective for E70CRL nuclear data library

Such a calibration is acceptable since the interpolation line between all cases is sufficiently horizontal and the linear correlation coefficient is sufficiently close to zero. Figure 11 reports the linear interpolation.

The calibration made at CRL for their simulations is assumed to encompass the correction of the quantity of poison dissolved in the moderator as well as all the model uncertainties.





Figure 11) Linear interpolation for adjusted boron cases for E70CRL data library (calibration)

# 5.2 Model calibration at ENEA

By contrast, the calculations carried out at ENEA utilized the ENDF/B-VII.1 nuclear data library. A second calibration – of the simulations made with the same MCNP input file but with different data – has been necessary. Starting at the nominal boron concentrations of case B4, a criticality search found that the poison concentration in the moderator has to be reduced by a factor of -19.75% (compared to -1.2% for E70CRL).



Figure 12) Calculation of k effective for cases in boron series: B1, B2, B4 and B4 with ENDF/B-VII.1 data

Results reported in Figure 12 are provided with uncertainties; they are not visible in the plot since the results are obtained with 1 pcm Monte Carlo statistical error at one standard deviation.



The horizontal line is required to attain a model calibration for the boron case. The nominal boron concentrations (blue dots) are far from a reference condition. The correction applied by the CRL research team in the calibration of the previous model is not sufficient (green dots). The adjustment applied by ENEA (red dots) reaches a calibration level, retained for the following steps.

We assume that the substantial difference in coefficients between the two calibrations is due in large part to the different cross-section libraries employed.

#### 6. Results and Comparisons

The aim of the present report is to verify the impact of newly measured gadolinium capture cross-sections for both <sup>157</sup>Gd and <sup>155</sup>Gd isotopes with corresponding data present in the ENDF/B-VII.1 set. It is known that currently employed data overestimate the capture reaction. Thus the plot in Figure 13 that shows the results obtained by the CRL research team demonstrates a clear underestimation of the multiplication coefficient. (The errors in the k effective values are shown with Monte Carlo statistical uncertainties of 6 pcm corresponding to 1 standard deviation).

The nominal concentrations in Table 1 are reduced to the adjusted concentration through the CRL calibration factor -1.2% to obtain the values reported in Table 4 obtained by CRL team.

Case	Adjusted Gd Conc. [ppm]	Critical Height [cm]	Multiplication Coefficient (keff)
Gadolinium G1	0.0	131.585	0.99788 ± 0.00006
Gadolinium G2	0.494	138.248	0.99766 ± 0.00006
Gadolinium G3	0.988	145.632	0.99759 ± 0.00006
Gadolinium G4	1.482	153.926	0.99713 ± 0.00006

Table 4) Gadolinium adjusted values and k effective for the E70CRL nuclear data library

The gadolinium results plotted in Figure 13 present some issues. If the gadolinium data in the E70CRL library were correct, the blue points should be aligned horizontally. Any correction which improves the gadolinium cross-sections is expected to modify the position of the points in the gadolinium series toward a horizontal distribution, or at least to a set of points on a line with a slope with a lower gradient. This statement is supported by the fact that a previous calibration has been made.

Therefore, simulations are performed with ENDF/B-VII.1 and with ENDF/B-VII.1 with <sup>157</sup>Gd substituted by the new measurements. This is performed under the following conditions:

- a) Concentration of the gadolinium poison is the nominal one shown in Table 1
- b) Concentration of the gadolinium poison is adjusted according to the CRL calibration: -1.2% (Table 4)
- c) Concentration of the gadolinium poison is adjusted according to the ENEA calibration: -19.75%

The hypothesis assumed is that the solubility of boron compound in heavy water is exactly the same as the gadolinium compound. This allows the utilization of the same coefficient to correct the concentration for both nuclides.



Figure 13) Calculation of k effective for Boron and Gadolinium (adjusted by CRL) for E70CRL data

case 3

case 4

case 2

case 1

The results for case (a) are reported in Figure 14, case (b) in Figure 15 and case (c) in Figure 16. Error bars provided present an uncertainty corresponding to one standard deviation. The errors reported in all three figures concern only the <sup>157</sup>Gd data since this is the only difference between the two simulations. The uncertainties of <sup>157</sup>Gd cross-sections - provided with the data set - are converted to error in k effective through a multiplication with the sensitivity coefficients of the system (scalar product made according to energy bins).



Figure 14) Comparison of standard ENDF/B-VII.1 and ENDF/B-VII.1 + <sup>157</sup>ENEA: nominal concentration



In the nominal case (Figure 14) from a situation in which the multiplication is underestimated, the simulation with ENEA <sup>157</sup>Gd new data tends to improve the behavior towards a horizontal line. The trend is consistent with a reduction in neutron capture. Multiplication factor in all cases evaluated with the new measured data is greater than the standard ENDF/B-VII.1 gadolinium data (without considering the error bars).



Figure 15) Comparison of standard ENDF/B-VII.1 and ENDF/B-VII.1 + <sup>157</sup>ENEA: CRL adjusted concentration



Figure 16) Comparison of standard ENDF/B-VII.1 and ENDF/B-VII.1 + <sup>157</sup>ENEA: ENEA adjusted concentration

Concerning case (b) in Figure 15 the two sets of results are almost symmetric with respect to the horizontal axis. In this case, it is difficult to state if the new data represent an improvement. Consideration of the error bars mitigates in any case against any firm conclusion.



Finally Figure 16 shows the case with the ENEA calibration with ENDF/B.VII.1 that was required to produce a horizontal line with boron in the moderator. Here the deviation from horizontal of the k effective values with the new <sup>157</sup>Gd data is greater than with standard ENDF/B.VII.1 data implying an even greater underestimation in the capture cross-section (although the error bars imply that no hard and fast conclusions can be drawn).

Simulations concerning <sup>155</sup>Gd similar to those shown in Figure 14, Figure 15 and Figure 16 have not yet been carried out. They are intended to be performed once a correct calibration methodology is established.

#### 7. Conclusions

Within the present report, the newly measured capture cross-sections for <sup>157</sup>Gd are considered after the sample irradiation campaign carried out at the n\_TOF facility at CERN by the ENEA and INFN research team. It is necessary to test the new data through numerical Monte Carlo simulations by means of MCNP6.1. Thus an experimental configuration is required that could have a thermal neutron spectrum and a significant presence of gadolinium poison. The ZED-2 nuclear research reactor at the Chalk River Laboratory (CRL) is considered since an experimental campaign has been carried out there with gadolinium to test the capture neutron cross-section. ZED-2 model data are obtained in the framework of the ENEA-IRSN collaborations.

In this document, some preliminary analyses are presented concerning the possibility to use ZED-2 as a benchmark, generating results with ENDF/B-VII.1 nuclear data library, then substituting <sup>157</sup>Gd with the new evaluation. The CRL research team that evaluated ZED-2 with the E70CRL in-house data library, at a particular temperature and moderator heights, provides the comparison and the reference data for ZED-2. They carried out also a model calibration procedure.

During this analysis the same calibration procedure employing well-known boron cross-sections, is performed. The poison concentration in the moderator is then adjusted and the same correction is applied to the gadolinium concentrations. Once the model is calibrated, ENDF/B-VII.1 reference data and ENDF/B-VII.1 with <sup>157</sup>Gd measured by ENEA are compared. The comparison is also performed with nominal concentrations and with the adjustment proposed by CRL team.

It seems that unfortunately, more details are necessary concerning the ZED-2 simulations before being able to state that this benchmark could provide information on the effects of the new data on the simulation. The temperatures of moderator and fuel as well as thermal scattering data should be considered in future simulations. In any case, it is worth remarking that the change of library from E70CRL to ENDF/B.VII.1 does not seem to be compensated by the calibration of the model through the correction of the boron concentration.

#### 8. Acknowledgments

Particular acknowledgement is given to Chalk River Laboratory (CRL) research team that provided ZED-2 input data and some references, as well as to Luiz Leal (IRSN) for the collaboration in testing newly measured nuclear data.

Authors would like to thank also Cristian Massimi, Gianni Vannini, Alice Manna, Giulia Clai and Alberto Ventura from the n\_TOF team of INFN/Bologna research team that carried out measurements, analysis and prepared the nuclear data evaluation.

The computing resources and the related technical support used for the MCNP calculations have been provided by CRESCO/ENEAGRID High Performance Computing infrastructure and its staff [10]. CRESCO/ENEAGRID High Performance Computing infrastructure is funded by ENEA, the Italian National Agency for New Technologies, Energy and Sustainable Economic Development and by Italian and European research programs, see http://www.cresco.enea.it/english for further information.



## 9. References

- [1] A. Guglielmelli et al., "Implementation of a Cross-sections Evaluation Methodology for Safety Margin Analysis: Application to Gadolinium Odd Isotopes", ENEA Report ADPFISS-LP1-083, 2016
- [2] International Criticality Safety Benchmark Evaluation Project (ICSBEP), Nuclear Energy Agency (NEA) database Reference to NEA webpage as follows: <u>https://www.oecd-nea.org/download/science/icsbephandbook/CD2018/</u>
- [3] D. Bernard, A. Santamarina, Ann. of Nucl. Eng., 87, 1 (2016)
- [4] D.M. Castelluccio and F. Rocchi, "Implementation of a Cross-section Evaluation Methodology for Safety Margins Analysis: Techniques and Experimental Campaign for New Evaluations of Neutron Capture Cross-sections of Gadolinium Odd Isotopes", ENEA Report ADPFISS-LP1-100, 2017
- [5] M. Mastromarco, A. Manna et al. (The n\_TOF Collaboration), "Cross section measurements of <sup>155,157</sup>Gd(n,γ) induced by thermal and epithermal neutrons", European Physical Journal A 55, 9 (2019)
- [6] J. Chow et al., "Nuclear Data and the Effect of Gadolinium in the Moderator", AECL Nuclear Review, 1 (2012), 21-25
- [7] D. Altiparmakov, "ENDF/B-VII.0 VERSUS ENDF/B-VI.8 IN CANDU<sup>®</sup> CALCULATIONS", PHYSOR Conference Proceedings, Pittsburgh, Pennsylvania, USA, May 9-14, 2010
- [8] G. Perret et al., 2009, "Impact of New Gadolinium Cross Sections on Reaction Rate Distributions in 10 × 10 BWR Assemblies", Nuclear Science and Engineering, 163, pp. 17 25
- [9] T. Goorley et al., "Initial MCNP6 Release Overview MCNP6 version 1.0", LA-UR-13-22934, (2013)
- [10] G. Ponti et al., Proc. of the 2014 International Conference on High Performance Computing and Simulation, HPCS 2014, 1030