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Numerical analysis of an incremented statistical sampling procedure in MCNP

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Abstract

MCNP has stood so far as one of the main Monte Carlo radiation transport codes. Its use, as any other Monte Carlo based code, has increased as computers perform calculations faster and become more affordable along time. However, the use of Monte Carlo method to tally events in volumes which represent a small fraction of the whole system may turn to be unfeasible, if a straight analogue transport procedure (no use of variance reduction techniques) is employed and precise results are demanded. Calculations of reaction rates in activation foils placed in critical systems turn to be one of the mentioned cases. The present work takes advantage of the fixed source representation from MCNP to perform the above mentioned task in a more effective sampling way (characterizing neutron population in the vicinity of the tallying region and using it in a geometric reduced coupled simulation). An extended analysis of source dependent parameters is studied in order to understand their influence on simulation performance and on validity of results. Although discrepant results have been observed for small enveloping regions, the procedure presents itself as very efficient, giving adequate and precise results in shorter times than the standard analogue procedure.

1. Introduction

Monte Carlo method based calculations have greatly increased along the years due to the steady development of the computational capabilities mainly regarding to the increment of memory handling and the decreasing of the processing time.

MCNP (Briesmeister, 2000; Brown et al., 2002) – Monte Carlo N Particle transport code stands for a long time, besides many other deterministic codes, as an important tool in the nuclear area. However, due to the aforementioned improvements in computing capabilities allied to its many other features, MCNP has turned to be an even more attractive instrument to perform radiation transport calculations.

However, as any Monte Carlo based codes, the quality of the results is dependent on the problem correct modeling as well as on the number of the interesting events recorded. The first point is related to the exactitude, i.e. how close does the tallied result get from the real one. Aiming at results with good exactitude demands the use of appropriate and reliable codes and data, and the correct problem modeling. Besides an up to date development, MCNP lays one of its most interesting features in its feasibility to describe geometrically any problem into a great detailed extent.

The second point is related to the precision of the result, i.e. how confident can anybody be about it. MCNP, similarly to any Monte Carlo code, stands as a simulated experiment and therefore its precision is dependent on the number of successful events tallied. The uncertainty decreases with the increment of these events and, in a straight forward manner, it can be made as small as desired as long as simulation keeps going on so that the desired value is reached.

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However, the $N^{-1/2}$ (inverse to the square root of the number of events) dependence of the uncertainty turns its procedure into an increasingly difficult task as uncertainty shrinks becoming even unfeasible from some point further. To circumvent this hurdle MCNP has a set of variance reduction techniques which aims, through special sampling or tally procedures, to improve precision without interfering in the exactitude of the result. The precise handling of these techniques is a very challenging task demanding quite some experience.

In the present work some situations in which the size of the tallied volume is some orders of magnitude lower than the simulated universe were faced with MCNP. A common procedure is either to decrease the size of the modeled universe or to enlarge the size of the tallying volume so to improve sampling efficiency. However, none of the procedures were taken in a straight forward way since the size of the tallying volume had already encompassed all the activation foils and a critical system was under consideration. Any attempt to change these modeling parameters was believed to affect result exactitude.

To overcome these time consuming simulations facing the above mentioned constraints a two step geometric sampling upgrade technique has been applied. It relies in a resource available in MCNP through the SSW and SSR cards. The first step consists in a short run of the entire system, thereby to well characterize the neutron population all over the system and principally recording this neutron population in the vicinity of the region of interest. The following step consists in running MCNP restricting the simulated region to coincide with the reduced one defined in the previous run.

This coupled simulation procedure, not exclusive to MCNP (Ma et al., 1997), is usually used to gain precision/time in tallying events in low (less than average) particle population density regions (Milgram, 1997; Ueki et al., 2003) or to avoid time consuming transport calculations through steady state systems (regions) from the source to its border (Ma et al., 1997; Coelho et al., 2002).

A great deal of difference of the proposition of this work rises at this point as this technique is usually used to speed up "outward simulations", simulations which can be divided in two distinct regions, and the tallied volume is away from the primarily source of particles. Here the tallying volume lies in a high particle population density region, immersed in the "primary source of particles". The conducted analysis, however, is believed to work on any case.

As the neutron population was characterized through the neutron recorded histories of the first run, these histories are used to permit running the second step in a geometric reduced fixed source simulating configuration. Doing so, the simulation runs faster than it does in the original way, due to the removal of particles which do not contribute to the tallied result and to the reduction of the particle's life span.

This is true even for a larger number of initial neutron histories, i.e. the number of simulated particles can exceed the number of recorded particles through their reuse at different point in the pseudo-random number sequence. It is also feasible to improve the precision of the calculated results through the continuous use of the fixed source with different pseudo-random sequences.

The present work describes some parameters sensitive studies in a coupled procedure performed to attain results with good precision avoiding long time demanding simulations. At first, however, a brief description of the problem is made followed by the description of the procedure itself. Results are then shown for some evaluated parameters before conclusion is presented.

2. The problem

Some of the work done by the reactor physics group of IPEN/CNEN-SP consists in performing experiments at the IPEN/MB-01 research reactor facility in order to support nuclear data evaluation and development of reactor physics calculation methods. The core of this facility consists of a 28×26 array of UO_2 fuel rods, 4.3% enriched and cladded by stainless steel (type 304) inside of a light water tank. A complete description of the IPEN/MB-01 reactor can be found in Dos Santos et al. (1999, 2004). One set of experiments performed at this facility was the $^{28}\rho$ and $^{25}\delta$ nuclear spectral indices evaluation. Nuclear spectral indices are defined as the ratio of epicadmium to subcadmium reaction rates, i.e. for a specific index it is given by the ratio of the related specific reaction promoted by neutrons with energies nearly above 0.625 eV by the same reaction promoted by neutrons with energies below that threshold. The motivations to perform such measurements in the IPEN/MB-01 core are the need of new and accurate measurements of such spectral indices for thermal reactor applications. Recently, in the framework of the Working Party in International Nuclear Data Evaluation and Co-operation (WPEC), it was reported a significant k_{eff} under-prediction (~ -500 pcm) (http://www.nea.fr/lists/ueval) with the most recent nuclear data libraries: ENDF/B-VI.8 (Rose, 2002), JENDL3.3 (Shibata et al., 2002) and JEFF3.0 (NEA, 2005), available in 2002. This underprediction was reported for a large set of independent integral experiments performed at various laboratories and using different experimental methods to measure criticality (variation of moderator height, control rod adjustment, critical boron technique, etc.). It was therefore assumed that the k_{eff} discrepancy was not due to common experimental error. Since independent Monte Carlo codes and processing methodologies were used, it was also assumed that the problem was not the consequence of approximations or errors in transport computer codes. Particularly to the ^{238}U nuclear data there have been found a k_{eff} bias as a function of ^{238}U capture fraction[1] (Kahler, 2003; Weinman, 2003). The analyses show a clear trend of decreasing k_{eff} with increasing ^{238}U capture fraction and this striking correlation was interpreted as an

[1] Ratio of ^{238}U capture rate over total absorption rate.

overestimation of the ^{238}U capture Shielded Resonance Integral (SRI). A literature survey shows that there is very few experimental support to serve as benchmark problems to verify the adequacy of the ^{238}U nuclear data. Many of them are not accurate enough to draw firm conclusions from. Similar trends with other integral parameters such as the above thermal fission fraction (ATFF) (Kahler, 2003) or the ^{235}U capture and fission fraction (Hanlon and Dean, 2003) were reported. Hence, it was argued that the observed trends might be attributable not only to ^{238}U but also to ^{235}U cross-section deficiencies. Consequently, the need of new and accurate measured integral parameters related to the ^{238}U and ^{235}U nuclear data such as $^{28}\rho$ and $^{25}\delta$ are desirable and completely acknowledged mainly regarding the very powerfull computational capabilities and the quality of the nuclear data libraries available nowadays.

Spectral Indices measurements have been performed in several facilities (Bitelli and Dos Santos, 2002; USAEC, 1974; Brown et al., 1967) by irradiation of bare cadmium covered depleted uranium foils. The common procedure was to use calculated correction factors (Sher and Fiarman, 1976; Bitelli and Dos Santos, 2002) to correct the cadmium and the aluminum foil perturbations and to convert the thermal cutoff to 0.625 eV. However, this procedure introduces unknown uncertainties due to the mathematical methods and nuclear data used in the determination of these correction factors. The proposed procedure in this work will be to calculate the spectral indices exactly as they were measured in the experimental approach and therefore simulating the real experiment. In the experiments two activations foils were placed inside one out of 680 fuel rods which make up the IPEN/MB-01 reactor core. The activations foils were located at different quotas inside a special dismountable fuel rod placed in the middle of core grid. Each one of these foils was sandwiched by Aluminum foils. At one of the chosen quotas a Cadmium sleeve was placed so to embrace the dismountable fuel rod. The axial positioning of the activation foils was made in such a way that the perturbation of the Cadmium sleeve to the bare position was minimal. ^{238}U neutron capture reaction and ^{235}U fission rates were evaluated for each of the activations foils to get respectively $^{28}\rho$ and $^{25}\delta$. The experimental work is still underway at the IPEN/MB-01 research reactor facility but some similar experimental results can be found in Bitelli et al. (2004).

MCNP has been used to simulate this experiment and to assess the simulated nuclear spectral indices gotten by using different nuclear data libraries. The hereinafter results are obtained by the ENDF-B.VI.8 processed by NJOY (MacFarlane et al., 1994), however the proposed methodology works with any nuclear data library and it is applicable to any critical system configuration in which tallied volumes are far smaller than the simulated universe.

3. The proposed procedure

Simulation starts by describing the entire universe of interest, i.e. the IPEN/MB-01 reactor core in its critical experimental configuration. Therefore, everything from the tiny activation foils up to the water tank which envelops the reactor core must be represented.

To simulate a critical system, MCNP provides a source information card known as KCODE which allows to represent a sustained chain reaction induced by fission neutrons. Successive neutron generations are represented by simulation cycles in which each neutron distribution source is characterized by the previous cycle, i.e. source distribution changes from cycle to cycle.

As the first generation source distribution is an user provided one, KCODE also allows the system to be stabilized before tally begins. It also controls how long simulation shall last. The higher the precision aimed the larger the number of particles histories to be followed. As the tallied volumes (approximately 4.5 mm^3) are very small compared to the size of the represented universe (approximately 2.6 m^3) a demand for a great number of histories is even more critical. For that reason allied to the need of waiting the stabilization of the system turn simulations to last long.

The first step records all particle histories which have crossed any chosen set of surfaces or have been created (fission neutrons) in specific volumes. SSW card is included in a regular run specifying all the selected surfaces and volumes whose related histories must be recorded. The second step uses the recorded file as a source specification for the particles to be generated. SSR card is used instead of the KCODE card and fission is turned off through the use of the NONU card. This second step has been conducted in a two fold procedure to account with the surface neutrons and fission neutrons separately. The final result is gotten from the sum of the results from both sources.

The simulation so approached turns the description of the system from a dynamical behavior, with particle histories of one cycle depending on the particle histories of the previous cycle (source description by KCODE card), to a static behavior, with all source information registered in a file (fixed source description). Therefore, there is no need to describe the whole system to tally a specific region since the particle population is already well characterized in the recorded file. Modeling a reduced universe of interest, embracing the tallied volume, samples a larger number of particle histories in a shorter time because time is not spent following unimportant particle histories, i.e. particles which do not play any role in the tally.

It does not represent any advantage just to rerun the simulation with the same number of histories ran in the first step. The prime benefit rests in increasing the number of histories so that each particle history recorded in the file is used many times but at a different point in the pseudo-random number sequence. It works similarly as a region with a higher particle importance in which a single particle history brings forth new particles with the same particle characteristics (even the same weight) at distinct points along the same pseudo-random number sequence. In addition to this source multiplication factor sampling increment the same source may be used again with different number sampling from the pseudo-random number sequence through different strides (the size of a number sequence reserved in advance to each particle generated from the source) number. It is done by using the DBCN card.

3.1. Does it work? How does it work?

As an example of the advantages of such procedure, the IPEN/MB-01 reactor was modeled and the ^{238}U Neutron Capture and ^{235}U Neutron Induced Fission reaction rates were tallied in a 10^4 cycles with 2.5×10^4 histories per cycle ($N\sim$ a quarter billion particle histories) MCNP run. In addition a fixed source was also created corresponding to reduced universe consisted of two boxes, each of them comprising a section of the nine innermost fuel rods and centered at the activation foil quotas.

Fig. 1a schematically shows the whole represented universe, i.e. the reactor core in the cylindrical water tank depicting the reduced universe in reactor core in order to give an idea of the related sizes. Fig. 1b–c show the top view cuts from both universes, the original and the reduced, and stress the zooming area to which the reduced universe is restricted.

Table 1 shows the tallied results and the related uncertainties (two last significant digits indicated between brackets) for ^{238}U neutron capture reaction and ^{235}U neutron induced fission obtained for both activation foils (in the same fuel rod at different quotas – one of them with a Cd sleeve surrounding the rod, whose results are identified by the letter W, and the other with no Cd sleeve, whose results are identified by the letter N) for distinct tally approaches:

- the original, in which the whole system (water tank and reactor core) is considered. It is the geometric description of the first step;
- the reduced universe proposal, in which a single run of a specific reduced universe system is considered (2 boxes, each of them comprising a section of the nine innermost fuel rods and centered at the activation foil quota). It constitutes the second step; and
- the repetition of the proposal, in which 84 simulations of the same reduced universe is ran and a mean value is taken as the final result and the uncertainty is obtained by the mean standard deviation. Fig. 2a–d shows the adequacy of such procedure as can be seen by the dispersion of data around their mean values, with roughly 3/4–2/3 of data comprising the mean value in their error bar.

Table 1 also shows the time demanded to run the simulations and an approximated number of particles (N) ran in

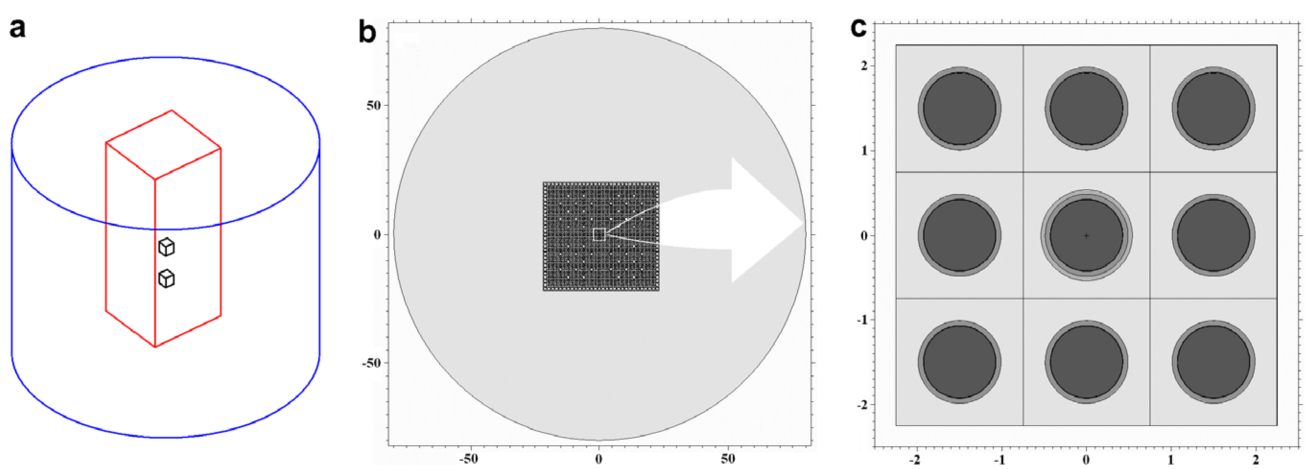

Fig. 1. (a) An overall representation of the original universe with the reactor core immersed in the water tank. The reduced universe is depicted in the reactor core; (b and c) a top view cut from the modeled universes. An arrow points out from a reactor central area to the reduced universe is zoomed out. Scales in the bottom and in the left of these figures give an idea o the related sizes.

Table 1
Simulated results and respective precision increments taking advantages from the above mentioned proposition

Procedure	N – Number of particles ($\times 10^9$)	Processing time (TU)	Cd	^{238}U neutron capture		^{235}U fission	
				Reaction/$n \cdot [^{238}\mathrm{U}]$ ($\times 10^{-4}$)	$^{28}\rho$	(Reaction/$n \cdot [^{235}\mathrm{U}]$) ($\times 10^{-3}$)	$^{25}\delta$
Original	0.25	53	W	4.02 (45)	2.4 (12)	3.72 (10)	0.1370 (52)
			N	5.71 (45)		30.84 (62)	
Reduced universe proposal	2.10	1	W	4.07 (20)	3.15 (75)	3.596 (33)	0.1277 (17)
			N	5.36 (17)		31.75 (22)	
Repetition of the proposal	$84 \times 2.10 = 176.40$	84	W	4.023 (17)	2.977 (62)	3.6559(45)	0.12962 (21)
			N	5.374 (16)		31.860 (25)	

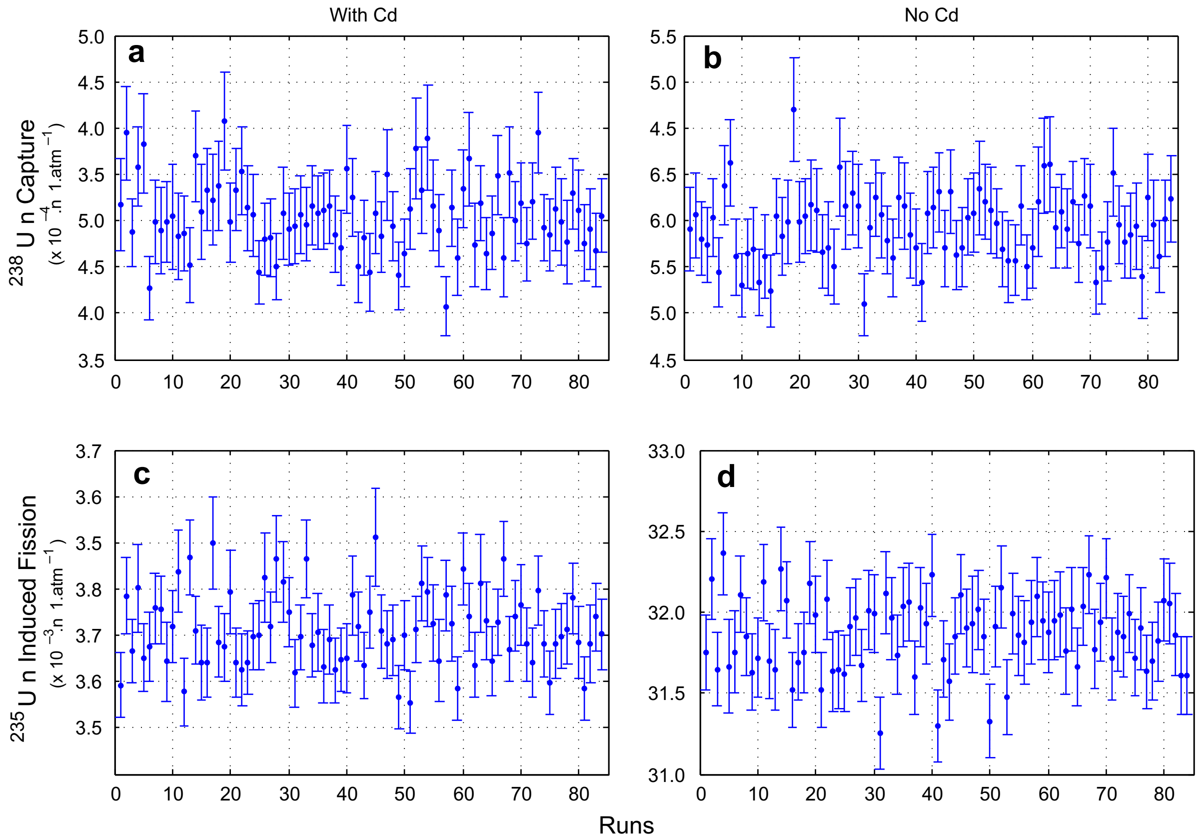

Fig. 2. Results from 84 reaction rates (a–b) ^{238}U neutron capture, (c)–(d) ^{235}U neutron induced fission) tallied for in each activation foil (a–c) embraced by a Cd sleeve, (b)–(d) not embraced by a Cd sleeve) by using reduced universe simulations.

the original procedure as each cycle has a slightly different number of particles. One can only control the number of cycles to be followed and the number of histories in the first cycle. Arbitrary time unity (TU) has been used, as processing time is dependent on computer facilities, operational system and on MCNP compilation options. These parameters points out to origin of the improvement in sampling efficiency as 8.4 more particles are followed in a much shorter time range (1/53) showing an enhancement of nearly 4.4×10^2 in sampling efficiency.

Reaction rates uncertainties were given either by the end of the simulation (original and reduced universe proposal) or by the mean standard deviation of the results (repetition of the proposal). Comparing the results from the original run with the reduced universe ones, one clearly sees a 1/3 reduction in the uncertainties, which stresses their $N^{-1/2}$ behavior, as the number of simulated particles increases almost 10 times.

Fig. 2 shows the reaction rates tallied results from each one of the 84 simulations run using the same fixed source. One can see that the individual uncertainties are of the same order from different simulations and which are of the same order of the statistical dispersion of the tallied results.

The uncertainties evaluated for the Repetition of the Proposal relies on the fact that the results from each simulation have all the same uncertainty, as they derive from the same distribution of results.

It is clear from the analysis of Table 1 the statistical compatibility of calculated results and the $N^{-1/2}$ decrease in their uncertainty. It also shows the nuclear spectral indices values obtained by each coupled results and as their uncertainties are proportional to their squared value it stresses the difficulty to shrink the $^{28}\rho$ uncertainty (not observed for $^{25}\delta$ as it is smaller than one).

4. The study

4.1. How precise?

The first aspect which may rise from this procedure is how far one can go in order to obtain more precise results, i.e. how many times one can reuse the recorded file to get more precise results.

At the first glance it seems this procedure could go over and more precise results could be gotten up to the point that a repetition in the pseudo-random number sequence would give rise to correlated results. However, the influence of the recorded file in the mean value should set a limit point in this precision eager procedure. In order to check the influence of the recorded file in the mean values, five other source files were created and 21 simulations were ran for each one of them. Table 2 and Fig. 3 show the results obtained. The reaction rates and their related spectral indices obtained from each of the new five sources, in spite of presenting distinct values, are statistically equivalent. The results not only agree in their attained values but also on their uncertainties as the number of followed particles are the same. The comparison of these results can be extended to the results of earlier 84 repetition of the proposed procedure. The results present statistically the same exactitude although the precision associated to

Table 2
Reaction rate means tallied for both activation foils (with Cd sleeve and No Cd sleeve surrounding the fuel element at the foil quota) and their respective spectral indices for five distinct fixed sources

Source files	Number of repetitions	Cd	^{238}U neutron capture		^{235}U fission	
			Reaction/$n \cdot [^{238}\mathrm{U}]$ ($\times 10^{-4}$)	$^{28}\rho$	(Reaction/$n \cdot [^{235}\mathrm{U}]$) ($\times 10^{-3}$)	$^{25}\delta$
a	21	W	4.000 (34)	2.94 (12)	3.6478 (74)	0.12925 (37)
		N	5.356 (28)		31.872 (49)	
b	21	W	3.995 (38)	2.94 (13)	3.6658 (51)	0.13013 (31)
		N	5.353 (31)		31.837 (51)	
c	21	W	4.016 (32)	3.11 (13)	3.650 (10)	0.12952 (46)
		N	5.305 (31)		31.828 (45)	
d	21	W	3.963 (31)	2.79 (10)	3.6422 (76)	0.12859 (38)
		N	5.383 (30)		31.966 (53)	
e	21	W	3.981 (39)	2.77 (11)	3.6604 (71)	0.12975 (34)
		N	5.418 (24)		31.872 (39)	
Original	84	W	4.023 (17)	2.977 (62)	3.6559 (45)	0.12962 (21)
		N	5.374 (16)		31.860 (25)	
Mean	$189 = 5 \times 21 + 84$	W	4.005 (11)	2.937 (39)	3.6544 (27)	0.12953 (13)
		N	5.368 (10)		31.868 (16)	

Mean values obtained for all sources are also presented at the bottom of the table together with the result previously shown.

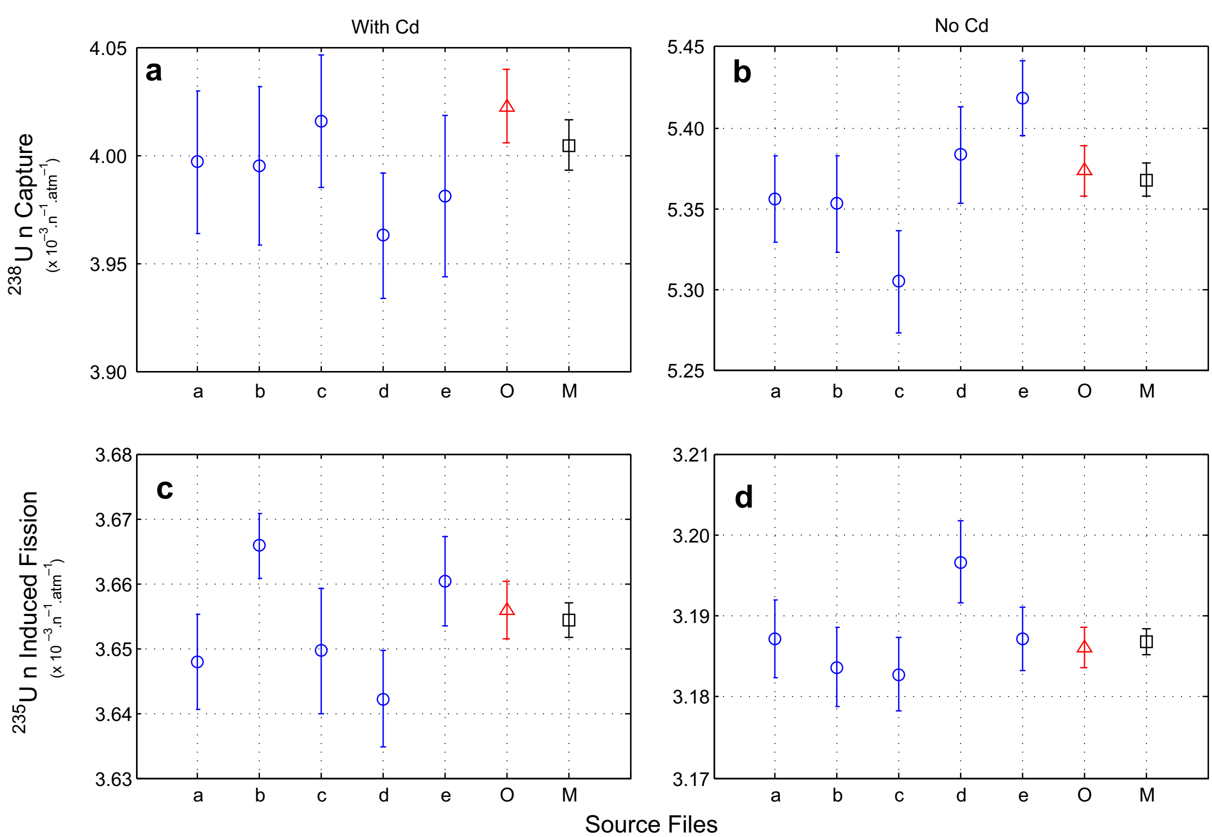

Fig. 3. Mean tallied reaction rates for each different used sources. Circles: mean out of 21 results. Triangle: mean out of 84 results. Square: mean out of 189 simulations. Top ones (a and b): ^{238}U n capture; bottom ones (c and d): ^{235}U n induced fission; left ones (a and c): with Cd sleeve surrounding the fuel rod; right ones (b and d): with no Cd sleeve.

the earlier one is half of those presented for these last five simulations due to a four fold larger number of particles. A mean value of all individual simulated outcomes is still presented. Fig. 4 shows the distribution of tallied results which supports the idea of a best value given by a mean value with an uncertainty given by the mean standard deviation.

4.2. Universe size

4.2.1. Geometric description

Another point which may rise from this procedure is how big should a reduced universe be, and what would be the advantages and disadvantages to take into account when optimizing the simulation. Therefore two other reduced universe descriptions were used to gain insight about these risen points.

- A larger reduced universe consisted of the nine most central core lattices at their full height, i.e. the nine fuel rods and the water contained in their respective lattices (see Fig. 5).

This large reduced universe is a longitudinal extension of the reduced universe so far used to somewhat all nine most central the fuel rods lattices.

- A smaller reduced universe consisted of 2 cylinders, 2 cm diameter and 5 cm high each, including the most central fuel rod (the one with the activation foils in it) and the water around it. One of the cylinders also comprised half of the 10 cm high Cadmium sleeve around the fuel rod. The cylinders diameter was chosen in such a way the maximum amount of water could be included in the cylinder without having to include any part of the neighboring rods (see Fig. 6).

This small reduced universe is a restriction of the transverse section of the reduced universe so far used (two segments of the nine most central fuel rods) to another circular section, centered along the dismountable fuel rod, embracing as much water as possible without "touching" another fuel rod.

Table 3 shows the mean values of the reaction rates followed through the present work obtained by an average of 84 repetitions of the three reduced universe sizes represented. In each repetition of the recorded source file, 2.1 billion histories were followed. Relative processing times are also presented in this table and although the demanded times may greatly differ (0.14–5, i.e. 35 folds), the outcomes from each different reduced universe source files have the same precision as they are derived from the same number of particles. It retakes the idea in which this procedure is

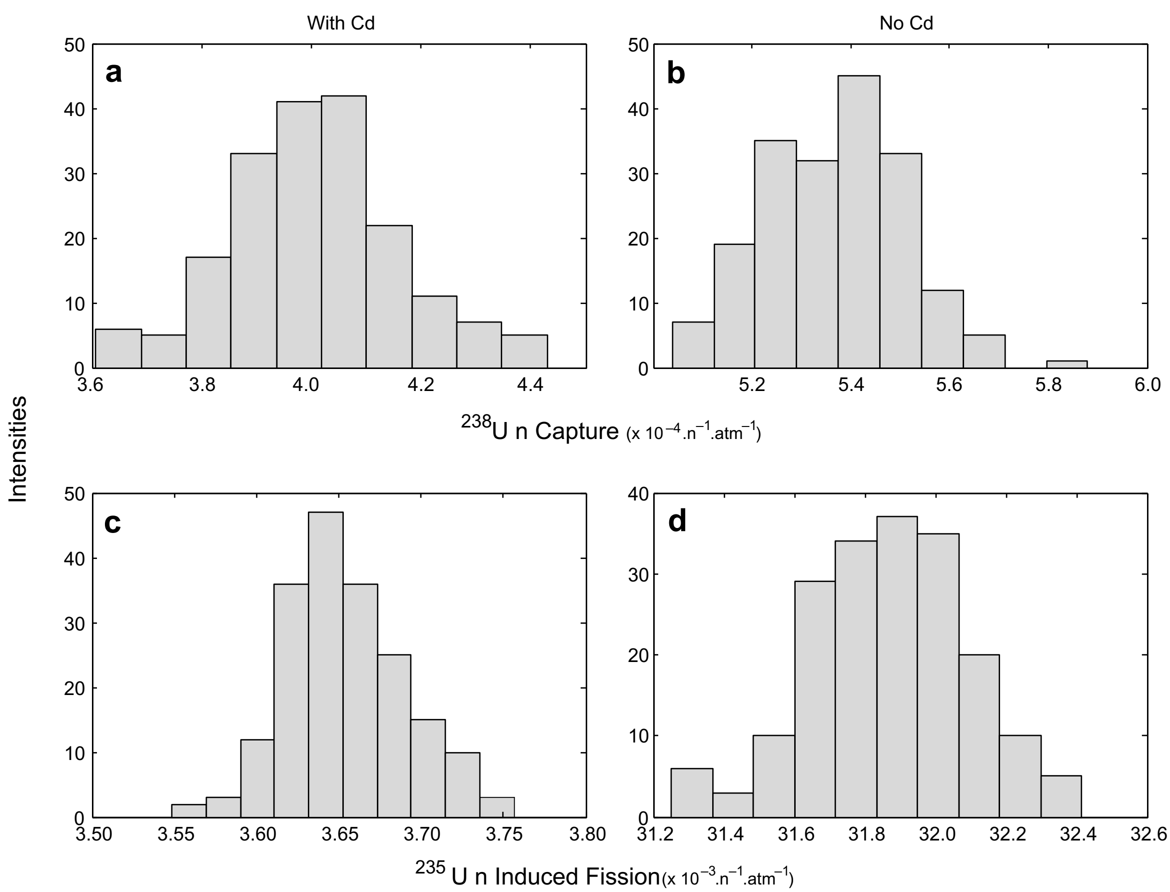

Fig. 4. Reaction rates distributions for tallied results obtained from 189 runs using 6 different fixed sources. Top ones (a and b): ^{238}U n capture; bottom ones (c and d): ^{235}U n induced fission; left ones (a and c): with Cd sleeve surrounding the fuel rod; Right ones (b and d): with no Cd sleeve.

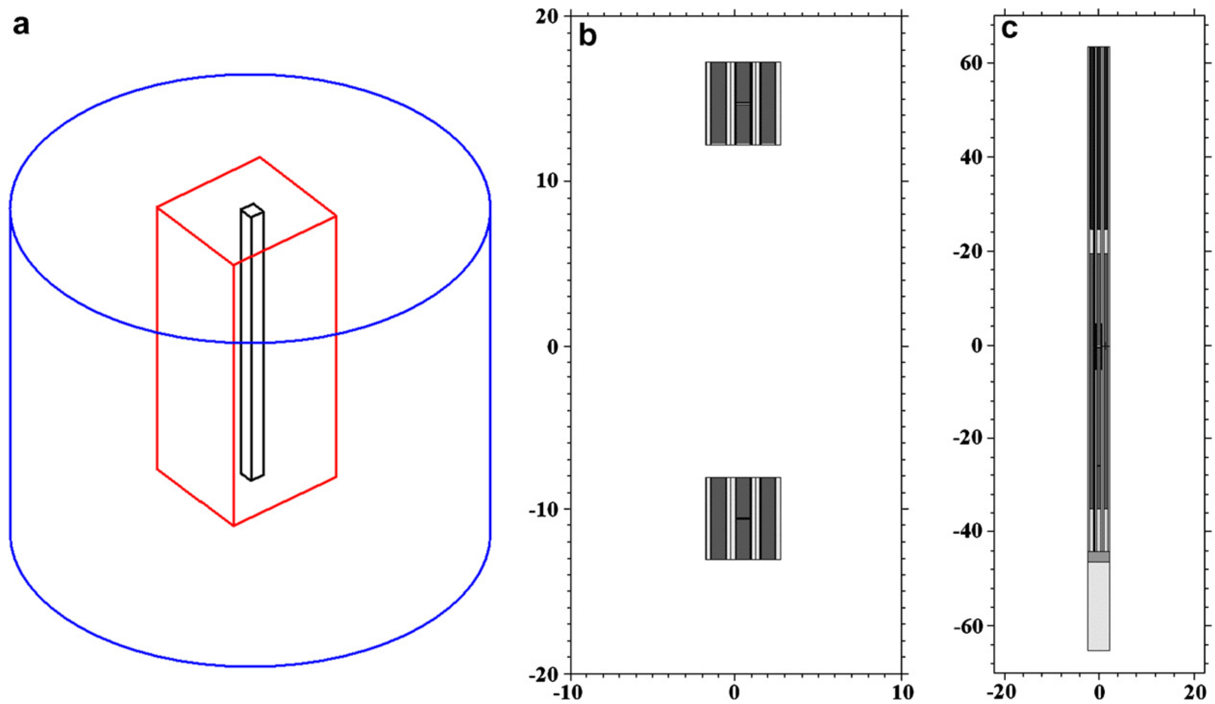

Fig. 5. (a) A schematic view of the larger reduced universe in the overall reactor. (b and c) A longitudinal 1–1 cuts of the original reduced universe (b) and the larger one (c). Scale labels (in cm) give an idea of the related sizes.

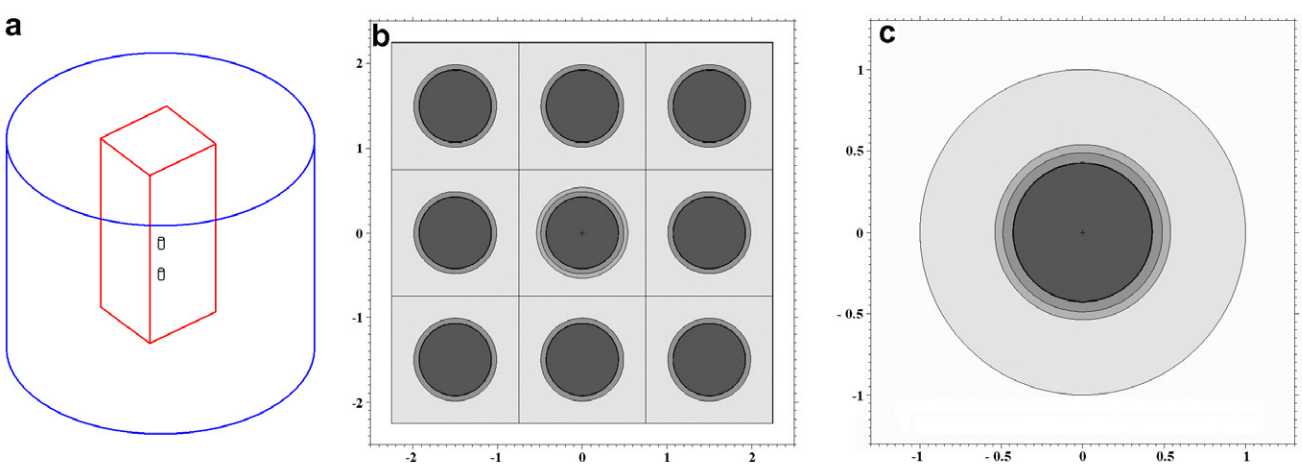

Fig. 6. (a) A schematic view of the small reduced universe in the overall reactor. (b and c) Top 1–1 cuts of the original reduced universe (b) and the smaller one (c). Scale labels give an idea of the related sizes.

Table 3
Reaction rate means tallied for both activation foils (with Cd sleeve and No Cd sleeve surrounding the fuel element at the foil quota) and their respective spectral indices using three different reduced universe representation

Reduced universe	Source file		Processing time (TU)	Cd	^{238}U neutron capture		^{235}U fission	
	Size (MB)	Particles recorded			Reaction/$n \cdot [^{238}U]$ ($\times 10^{-4}$)	$^{28}\rho$	(Reaction/$n \cdot [^{235}U]$)($\times 10^{-3}$)	$^{25}\delta$
Large	716	6.35×10^6	5	W	3.995 (17)	2.833 (60)	3.6450 (41)	0.12863 (20)
				N	5.405 (19)		31.983 (25)	
Medium	895	8.56×10^6	1	W	4.023 (17)	2.977 (62)	3.6559 (45)	0.12962 (21)
				N	5.374 (16)		31.860 (25)	
Small	238	2.04×10^6	0.14	W	4.154 (17)	3.394 (75)	3.5921 (30)	0.12890 (17)
				N	5.378 (16)		31.460 (25)	

Table 4
Reaction rate means tallied for both activation foils (with Cd sleeve and No Cd sleeve surrounding the fuel element at the foil quota) and their respective spectral indices for four distinct fixed sources sizes obtained for the medium size reduced universe

Number of cycles	Source file		Source multiplication	Cd	^{238}U neutron capture		^{235}U fission	
	Size (MB)	Particles recorded			Reaction/$n \cdot [^{238}\text{U}]$ ($\times 10^{-4}$)	$^{28}\rho$	(Reaction/$n \cdot [^{235}\text{U}]$) ($\times 10^{-3}$)	$^{25}\delta$
1900	170	1.63×10^6	44.2	W	3.958 (41)	2.64 (11)	3.6402 (74)	0.12924 (35)
				N	5.455 (26)		31.807 (41)	
10,000	895	8.56×10^6	8.4	W	4.074 (40)	3.19 (16)	3.6575 (97)	0.12966 (47)
				N	5.353 (39)		31.866 (59)	
15,800	1415	1.35×10^7	5.3	W	3.979 (32)	2.96 (11)	3.6425 (68)	0.12898 (35)
				N	5.325 (28)		31.884 (47)	
20,800	1862	1.78×10^7	4.0	W	3.975 (32)	2.83 (11)	3.6326 (70)	0.12869 (36)
				N	5.380 (30)		31.861 (49)	

Table 5
Reaction rate means tallied for both activation foils (with Cd sleeve and No Cd sleeve surrounding the fuel element at the foil quota) and their respective spectral indices for five distinct fixed sources sizes obtained for the small size reduced universe

Number of cycles	Source file		Source multiplication	Cd	^{238}U neutron capture		^{235}U fission	
	Size (MB)	Particles recorded			Reaction/$n \cdot [^{238}\text{U}]$ ($\times 10^{-4}$)	$^{28}\rho$	(Reaction/$n \cdot [^{235}\text{U}]$) ($\times 10^{-3}$)	$^{25}\delta$
1900	45	3.86×10^5	44.2	W	3.670 (36)	2.54 (10)	3.6592 (62)	0.13103 (28)
				N	5.117 (25)		31.586 (26)	
10,000	239	2.04×10^6	8.4	W	4.213 (31)	3.54 (17)	3.5850 (56)	0.12835 (31)
				N	5.402 (39)		31.516 (46)	
20,800	496	4.24×10^6	4.0	W	4.004 (34)	2.93 (14)	3.5754 (60)	0.12869 (33)
				N	5.370 (47)		31.359 (48)	
39,800	949	8.59×10^6	2.1	W	3.979 (29)	3.21 (16)	3.5251 (53)	0.12962 (34)
				N	5.219 (47)		30.721 (54)	
59,800	1426	1.22×10^7	1.4	W	3.849 (40)	3.17 (16)	3.4413 (56)	0.12981 (35)
				N	5.064 (30)		29.951 (52)	

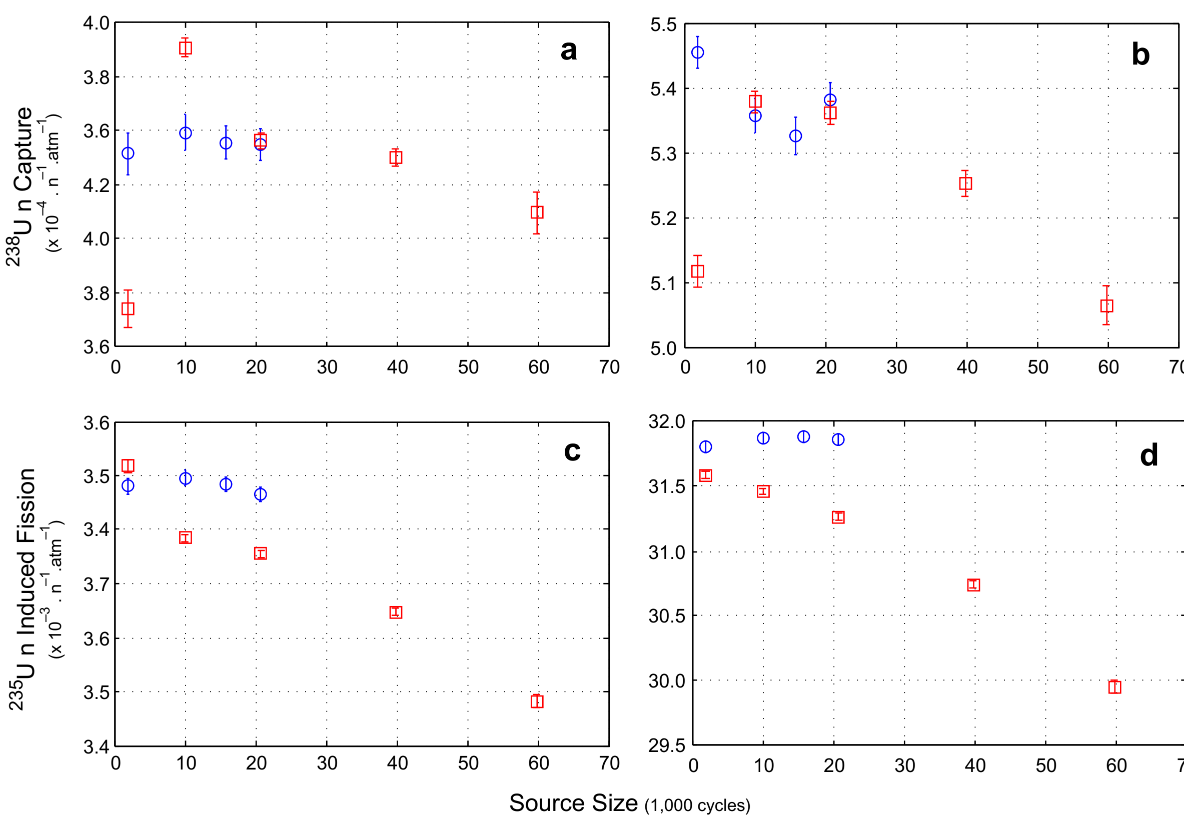

Fig. 7. Dependence of the mean calculated simulation rates with source sizes (number of cycles in the original run) for 2 distinct reduced universe sizes (circle: medium; square: small). Top ones (a and b): ^{238}U n capture; bottom ones (c and d): ^{235}U n induced fission; left ones (a and c): with Cd sleeve surrounding the fuel rod; right ones (b and d): with no Cd sleeve.

laid on, the improvement in sampling efficiency rather than reducing the variance of the tallied events.

It is also shown, in Table 3, the size of the recorded files created and used to run the simulations in their reduced universe representation. At this point a remark shall be made: the number of cycles for the largest reduced universe representation is five fold smaller than the other two representations. Fewer cycles were followed for the large reduced universe in order to avoid the creation of an extreme large source file. This point drives attention to an important point in which this procedure is laid on: the source file. For a fixed number of cycles the larger the reduced universe representation, the larger the source file created. As recorded file sizes are of the order of thousands of MB for typical cases (e.g. 1900 cycles with 25,000 histories/cycle for the large reduced universe representation), file manipulation and computer availabilities should be taken into account before creating a source file.

Processing time and source size seem to push to a "smaller the best" choice for a reduced universe representation. However, a closer look at the simulated results shows an incompatibility among them. Except for the ^{238}U neutron capture in the activation foil not covered by the Cd sleeve, all reaction rates results differ for the small reduced universe representation. An intriguing result comes from de $^{25}\delta$ value obtained for the small universe representation. It looks to be in accordance to the ones gotten by the others reduced universe representation despite the differences observed for the simulated ^{235}U neutron induced fission rates.

4.3. Number of cycles

Another point which has been checked about the record file is its size. Criticality simulations with different number of cycles were carried out to generate files with different amounts of recorded particles. The same original reduced universe (delimiting planes and included volumes) was used in subsequent set of fixed source simulations. Table 4 shows different sources sizes parameters and their related reaction rates mean values obtained for a set of 21 repetitions with a medium size universe representation while Table 5 shows the same parameters gotten with a small universe representation. The reaction rate data from these two tables are merged in Fig. 7.

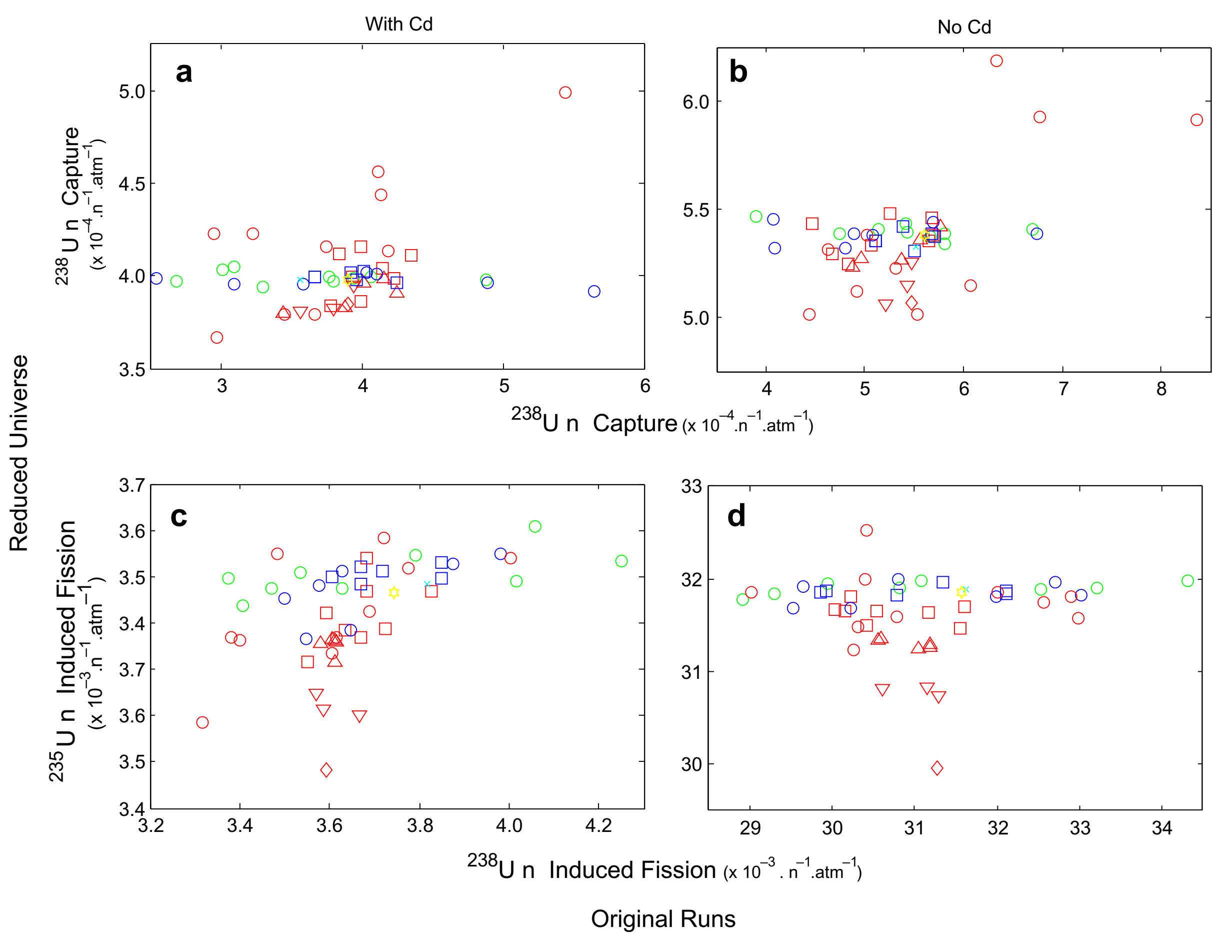

Fig. 8. Mean tallied reaction rate values obtained from reduced universe simulations using diverse source and universe sizes versus the outcomes of the original runs performed in order to generate the sources used. Top ones (a and b): ^{238}U n capture; bottom ones (c and d): ^{235}U n induced fission; left ones (a and c): with Cd sleeve surrounding the fuel rod; right ones (b and d): with no Cd sleeve. Reduced universes: green: large; blue: medium and red: small. Source size: circle: 2 kc; square: 10 kc; triangle: 20 kc; up side down triangle: 40 kc and diamond: 60 kc.

Tables 4 and 5 show the linear growth of source file size with the number of cycles recorded during the critical system simulation. Processing time has been omitted from the tables as it does not dependent on the number of cycles, but tightly on the geometric size of the reduced universe representation. On the other hand, time demand for creating file simulation does obviously dependent on the number of cycles followed.

Source multiplication factor indicates how many times a recorded particle is used to run a 2.1×10^9 particle histories fixed source simulation. Although only the recorded particles are used during fixed source simulation MCNP uses the number of particles histories followed in the criticality case simulation to normalize the tallying parameters and to set the multiplication factor.

Simulated reaction rates for the medium reduced universe representation do not seem to present any dependence on source cycle size as all values are in statistical accordance. This is not the true for the small reduced universe representation as its reaction rate estimates do not present a statistical agreement, showing a decreasing trend with the increment of number of cycles from some point on.

5. Panoramic idea

In order to get an idea of the reproducibility/stiffness of these results many other fixed sources were generated and a set of 21 fixed source simulations were carried out.

Fig. 8 shows the plot of ^{238}U neutron capture and ^{235}U neutron induced fission mean values obtained from each set of 21 reduced universe simulations against their associated values tallied in original runs performed to create the source files. As was observed in Fig. 3 there is no dependence of the reduced universe simulation results on coupled source generation simulations. As would be expected, the larger the number of cycles in the original run the smaller the dispersion of the tallied values obtained through the simulations carried to create the source files.

In order to facilitate its reading, Fig. 8d can stand as the reference plot to follow the commentaries: for the smallest sources created (~2000 cycles in the Original runs), the Small reduced universe simulations yield very disperse results, which are statistically inconsistent. Although this behavior seems to disappear as the source file size increases, the mean values obtained drift to lower values thereafter. This trend shows the inadequacy of the

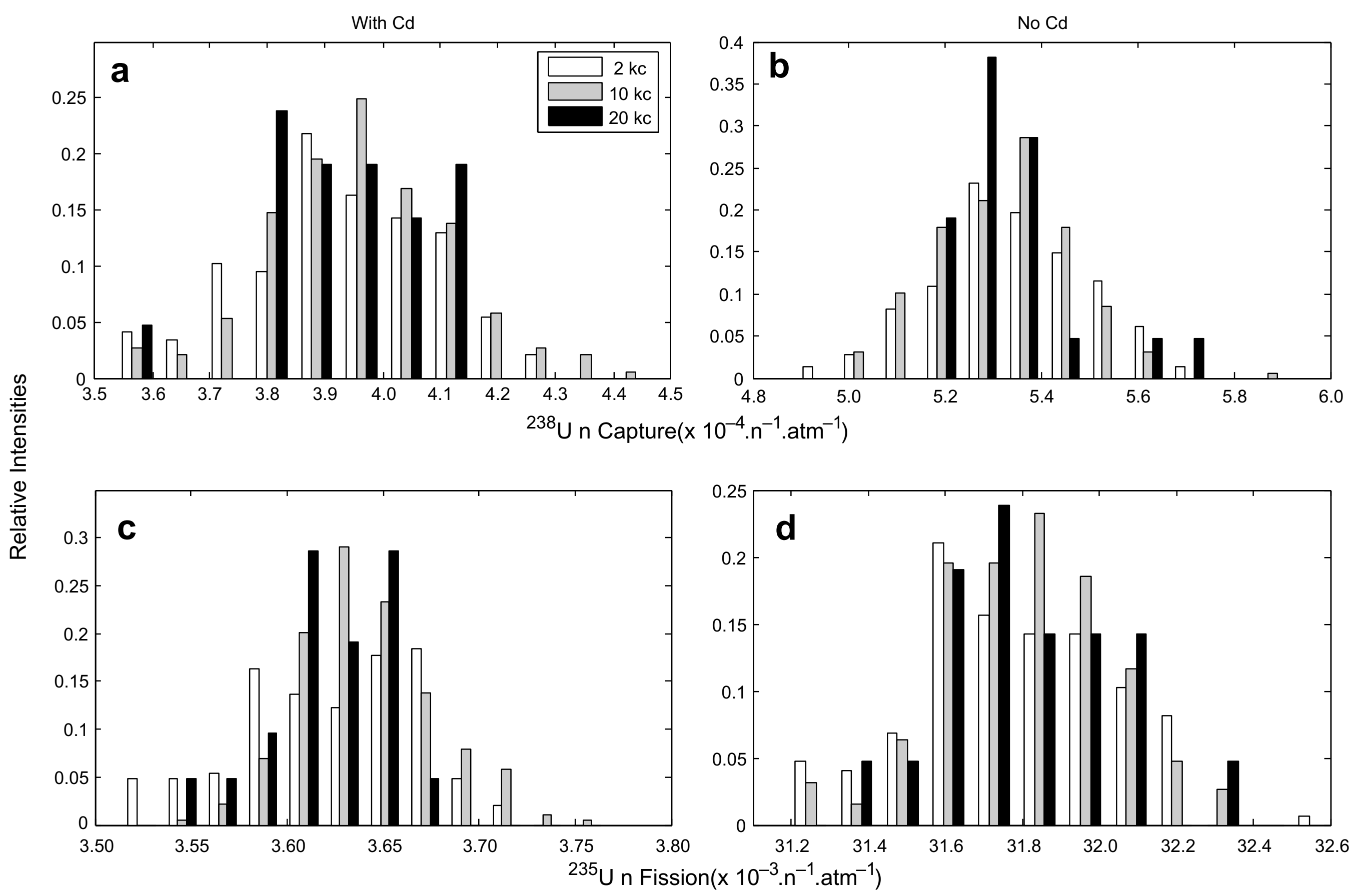

Fig. 9. Histograms of reaction rates (a–b ^{238}U neutron capture, c–d ^{235}U neutron induced fission) obtained in each activation foil (a–c embraced by a Cd sleeve, b–d not embraced by a Cd sleeve) for the medium reduced universe representation sorted by the number of cycles followed.

small reduced universe representation to assure reliable results, suggesting a minimum representation limit to proposed procedure. The existence of such limit to the appliance of this procedure was already expected as a minimal amount of interactions shall occur so that multiple uses of the same recorded particle do not lead to correlated tallied events. The intriguing fact is the fall down of the premise the larger the source file the better characterized it is. On the other hand, mean values obtained through the large and medium reduced universes fixed sources, are concentrated in narrower ranges showing consistent results and no dependence on the number of the cycles of the coupled source generation simulation, evidencing the adequacy of the used methodology.

Fig. 9 reinforces the fact that for medium reduced universe representation the tallied values obtained for the adopted procedure do not depend neither on specific criticality case run nor on number of cycles followed in order to create the source file.

Therefore all results can be assembled together. Fig. 10, on the other hand, shows the dependence of the tallied result on the number of cycles, reinforcing the idea of Fig. 7. It also stresses the feasibility to join the data obtained from different sources with same size (geometric and number of cycles).

Table 6 shows the final results obtained by all fixed source simulations divided into reduced universe representation, except for the small reduced universe where results were subdivided in source files cycles sizes. It is also includes a result obtained by gathering all independent results presented in each criticality simulation run to create the fixed source files. More than 3×10^5 cycles ($N > 7.5 \times 10^9$ particles) were computed to get the associated values. Table 6 also presents, in arbitrary units, the processing time taken in the whole procedure to get such results. Right below, the associated fraction of this time spent running the fixed source simulations. These time data should be read with care as the number of fixed sources created varied in each set as well as did the number of fixed sources simulations. Nonetheless, they illustrate the role played by the studied procedure in processing time demand.

It is clear from the analysis of Table 6 the improvement in results precision when taking the fixed source simulation with even a reduction in processing time.

Taking the 3 σ's ranges obtained from the "whole system" representation, i.e. the critical simulation, as limit values to encompass the target values, only the results from the Large and Medium universe representations would meet this criterion. Small reduced universe representation

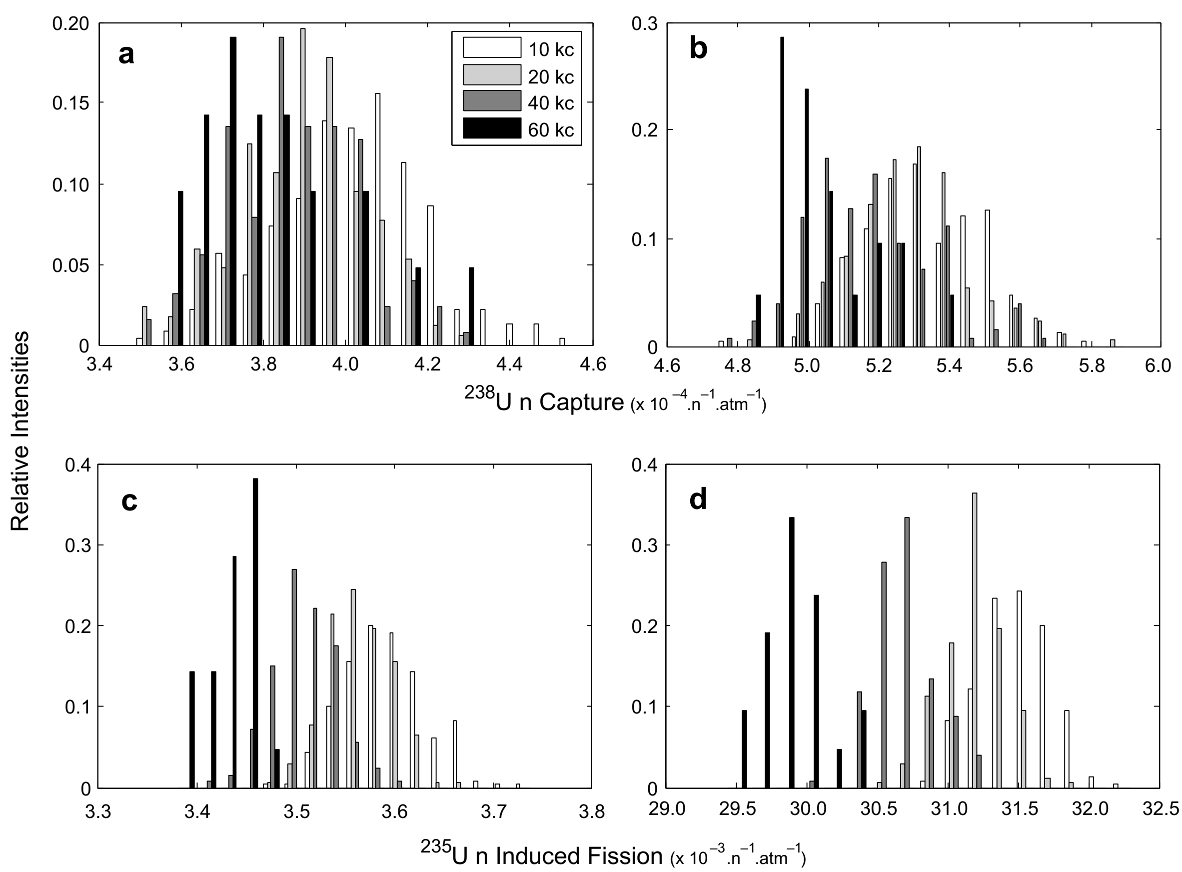

Fig. 10. Histograms of reaction rates (a–b ^{238}U neutron capture, c–d ^{235}U neutron induced fission) obtained in each activation foil (a–c embraced by a Cd sleeve, b–d not embraced by a Cd sleeve) for the small reduced universe representation sorted by the number of cycles followed.

Table 6
Final results

Reduced universe representation		Relative processing time	Cd	^{238}U neutron capture		^{235}U fission	
				Reaction/$n \cdot [^{238}U]$ ($\times 10^{-4}$)	$^{28}\rho$	(Reaction/$n \cdot [^{235}U]$) ($\times 10^{-3}$)	$^{25}\delta$
Large		2.2 (93%)	W	3.995 (10)	2.841 (33)	3.6528 (20)	0.12919 (10)
			N	5.401 (9)		31.928 (14)	
Medium		1.0 (37%)	W	4.000 (10)	2.909 (34)	3.6579 (17)	0.12918 (7)
			N	5.375 (9)		31.975 (26)	
Small	1900 cycles	0.2 (21%)	W	4.175 (11)	3.615 (52)	3.6204 (20)	0.12886 (60)
			N	5.330 (9)		31.716 (12)	
	10,000 cycles	0.7 (7%)	W	4.056 (9)	3.094 (37)	3.6090 (19)	0.12893 (8)
			N	5.367 (10)		31.600 (15)	
	20,800 cycles	0.9 (3%)	W	3.891 (14)	2.769 (48)	3.5746 (30)	0.13020 (12)
			N	5.296 (15)		31.030 (22)	
	39,800 cycles	2.1 (4%)	W	3.875 (17)	3.123 (76)	3.5132 (36)	0.12879 (15)
			N	5.114 (20)		30.792 (30)	
	59,800 cycles	1.0 (1%)	W	3.849 (40)	3.17 (16)	3.4413 (56)	0.12981 (35)
			N	5.064 (30)		29.951 (52)	
Whole System		2.5 (0%)	W	3.76 (7)	2.52 (21)	3.664 (18)	0.1296 (9)
			N	5.26 (8)		31.93 (12)	

fails to accomplish it as ^{238}U neutron capture in the covered activation foil stands higher above it for the 10,000 cycles and the ^{235}U neutron induced fission in both activation foils stand far below it for the remaining sources.

This failure added to presented drift of tally values with source file size turns the small reduced universe into an unreliable representation. Anyway the results obtained by the large and medium universe representations behave in accordance to what is expected and seems to present reliable results.

6. Conclusions

A straightforward approach to calculate the reaction rates in activations foils placed in a critical configuration system may become too time consuming, practically unfeasible, if precise results are sought. The use of fixed source files to enhance statistical sampling in tiny talling volumes in such systems stands as a very promising approach as 2–3 orders of magnitude more particles can be simulated in the same time frame, with a trend to "the smaller the represented reduced universe more particles are followed". A check of the stability of results shall, however, be made to assure the exactitude of the result.

Time savings can be made both reducing the geometric representation of the reduced universe as on the increment of the multiple use of the same fixed source. No advantage associated to the enlargement of the source file, i.e. following an increased number of cycles in the coupled source generation simulation, has been observed for the studied cases except for the check of consistency of the results.

The use of a set of fixed source generated by a smaller number of cycles (histories) rather than a single fixed source generated by the same total number of cycles (histories) is preferable, as the amount of time spent to generate them are quite the same and not only small file manipulation are easier (writing, reading and storing) but a more precise final result is attained. Nonetheless, it is worthy to extend the number of cycles to at least one of the source files to check the stability of the results.

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References

Bitelli, U., Dos Santos, A., 2002. Experimental determination of the spectral indices $^{28}\rho$ and $^{25}\delta$ of the IPEN/MB-01 reactor. Journal of Nuclear and Science Technology 2, 932–935.

Bitelli, U., Dos Santos, A., Jerez, R., Fanaro, L.C., Cacuri, R.R., 2004. The experimental determination of the spectral indices ρ-28 and δ-25 inside of the fuel pellet of the IPEN/MB-01 reactor. In: International Conference on Nuclear Data for Science and Technology, Santa Fe, NM, USA, September 28–October 1.

Briesmeister, J.F. (Ed.), 2000. MCNP – A General Monte Carlo N-Particle Code, Version 4C, Technical Report LA-13709-M, Los Alamos National Laboratory, USA.

Brown, W.A.V., Fox, W.N., Skillings, D.J., George, C.F., Burholt, G.D., 1967. Measurements of material buckling and detailed relation rates in a series of low enrichment UO_2 fuelled cores moderated by light water. AEEW – R502.

Brown, F.B., Barrett, R.F., Booth, T.E., Bull, J.S., Cox, L.J., Forster, R.A., Goorley, T.J., Mosteller, R.D., Post, S.E., Prael, R.E., Selcow, E.C., Sood, A., Sweezy, J., 2002. MCNP Version 5, LA-UR-02-3935.

Coelho, P.R.P., Hernandes, A.C., Siqueira, P.T.D., 2002. Neutron flux calculation in a BNCT research facility implemented in IEA-R1 reactor. In: Wolfgang, S., Raymond, M., Andrea, W. (Eds.), Research and Development in Neutron Capture Therapy. Monduzzi, Bologna, pp. 197–201.

Dos Santos, A., Pasqualeto, H., Fanaro, L.C.C.B., Fuga, R., Jerez, R., 1999. The inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor-1: experimental procedure. Nuclear Science and Engineering 133, 314–326.

Dos Santos, A., Fanaro, L.C.C.B., Yamaguchi, M., Jerez, R., Silva, G.S.A., Siqueira, P.T.D., Abe, A.Y., Fuga, R., 2004. LEU-COMP-THERM-077 critical loading configurations of the IPEN/MB-01 reactor. In: BlairBriggs, J. (Ed.), International Handbook of Evaluated Criticality Safety Benchmark Experiments, NEA/NSC/DOC (95)03/I. Nuclear Energy Agency, Paris.

Hanlon, D., Dean, C., (2003). communication to ueval forum, http://www.nea.fr/sympa/arc/ueval/2003-04/msg00001/jefdoc-950.pdf.

Kahler, A.C., 2003. Monte carlo eigenvalue calculations with ENDF/B-VI.8, JEFF-3.0, and JENDL-3.3 cross sections for a selection of international criticality safety benchmark evaluation project handbook benchmarks. Nuclear Science and Engineering 145, 2.

MacFarlane, R.E., Muir, D.W., Bouicort, R.M., 1994. NJOY – code system for producing pointwise and multigroup neutron and photon cross sections from ENDF data. LA-12740-M, Los Alamos National Laboratory.

Ma, C.M., Faddegon, B.A., Rogers, D.W.O., Mackie, T.R., 1997. Accurate characterization of Monte Carlo calculated electron beams for radiotherapy. Medical Physics 24 (3).

Milgram, M.S., 1997. Estimates of the neutron flux distribution in an end-fitting of bruce unit 2 using MCNP. In: Joint International Conference on Mathematical Methods and Supercomputing for Nuclear Applications, Saragota Springs.

NEA – Nuclear Energy Agency, 2005. The JEFF-3.0 Nuclear Data Library, JEFF Report 19, Synopsis of the General Purpose File, NEA No. 3711.

Rose, P.F. (Ed.), 2002. ENDF/B-VI Summary Documentation, BNL-NCS-17541 (ENDF-201), fourth ed. (ENDF/B-VI), National Nuclear Data Center, Brookhaven National Laboratory, Release-8.

Sher, R., Fiarman, S., 1976. Studies of thermal reactor benchmark data interpretation: experimental corrections, Standford University, Standford.

Shibata, K. et al., 2002. Japanese evaluated nuclear data library version 3 revision-3: JENDL3.3. Journal of Nuclear Science Technology 39, 1125.

Ueki, K., Kawakami, K., Shimizu, D., 2003. Using the Monte Carlo coupling technique to evaluate the shielding ability to a modular shielding house to accommodate spent-fuel transportable storage casks. Nuclear Technology 141, 177–185.

USAEC – United States Atomic Energy Commission, 1974. Cross Section Evaluation Working Group Benchmark Specification, USAEC Report BNL 19302 (ENDF-202).

Weinman, J.P., 2003. Communication to ueval forum, http://www.nea.fr/sympa/arc/ueval/2003-01/msg00001.html.