2011 International Nuclear Atlantic Conference - INAC 2011
Belo Horizonte,MG, Brazil, October 24-28, 2011
ASSOCIAÇÃO BRASILEIRA DE ENERGIA NUCLEAR - ABEN
***ISBN:* 978-85-99141-04-5**

A STOCHASTIC MODEL FOR NEUTRON SIMULATION CONSIDERING THE SPECTRUM AND NUCLEAR PROPERTIES WITH CONTINUOUS DEPENDENCE OF ENERGY

Dayana Q. de Camargo[1], Bardo E.J. Bodmann [1], Marco T. de Vilhena[1] and Sergio de Q. B. Leite[2], Herberth B. Fröhlich[1]

[1] Departamento de Engenharia Mecânica
Universidade Federal do Rio Grande do Sul
Rua Sarmento Leite, 425
90050-170 Porto Alegre, RS
dayanadecamargo@gmail.com
bejbodmann@gmail.com
vilhena@mat.ufrgs.br
hbfmec@gmail.com

[2] Comissão Nacional de Energia Nuclear
Rua General Severiano, 90
22294-900 Rio de Janeiro, RJ
bogado@cnen.gov.br

ABSTRACT

In this work we developed a stochastic model to simulate neutron transport in a heterogeneous environment, considering continuous neutron spectra and the nuclear properties with its continuous dependence on energy. This model was implemented using the Monte Carlo method for the propagation of neutrons in different environments. Due to restrictions with respect to the number of neutrons that can be simulated in reasonable computational time we introduced a variable control volume together with (pseudo-) periodic boundary conditions in order to overcome this problem. This study allowed a detailed analysis of the influence of energy on the neutron population and its impact on the life cycle of neutrons. From the results, even for a simple geometrical arrangement, we can conclude that there is need to consider the energy dependence and hence defined a spectral effective multiplication factor per Monte Carlo step.

1. INTRODUCTION

Controlled nuclear reactions in a nuclear reactor is an energy resource that can contribute to meet the growing demand for electric energy while minimizing the impact on the environment. Because of its efficient liberation of energy by nuclear reactions, the control and safety of reactors is a crucial issue. When designing new reactor concepts, the microscopic, and the macroscopic nuclear processes must be understood in detail and adequately described in terms of mathematical models together with experimental data, such as cross sections of the relevant nuclear reactions [5,6].

The experience acquired along the nuclear history has reinforced the rules and regulations that lead to the commissioning of next generation nuclear technology. One question is the exploration of physical laws in favor of the control of the reactor. Although there is a variety of aspects that should be taken into account, this paper focuses on the question of the influence of the energy spectrum of neutrons, and of nuclear properties, with its continuous

energetic dependence in a stochastic model that simulates the neutron transport. The energetic dependence is therefore the main progress compared to approaches that make use of energy groups, often only two, the fast and thermal group.

The physics of nuclear reactions that occur in a power reactor, and its influence on the flux of neutrons by disturbances from inside or outside the system are reasonably well known, but there is still much to be studied. One knows very well the flow of neutrons in the case where energy dependence is simplified by the use of multigroups of energy. However, the influence of a continuous energy dependence in the behavior of neutrons, and physical quantities important in studies of reactors, is still poorly explored. With the present contribution we show that there is still room for progress. A variety of recent attempts to create appropriate and efficient algorithms for calculating the populations of neutrons, and other relevant quantities in calculations of nuclear reactors is a manifestation of that fact.

In this work, the Monte Carlo implementation [3,8] takes its instructions from an integro-differential neutron transport equation, in three dimensions and with true energy dependence. Here the cross sections are continuous functions of energy, and are obtained by parameterizations and coded as program procedures. The type of interaction that a neutron will suffer, and the characteristics of their displacement in the environment, are randomly estimated by use of relevant probability distributions.

In order to make the simulation efficient, the medium is divided into several smaller volumes, where these volumes are selected and play the role of control volumes. These small volume elements are chosen to reconstruct the smooth distribution of neutrons to the entire volume. Its advantage is that the number of neutrons can be significantly reduced, while still getting a satisfactory simulation. In this paper it is shown how the method works together with first results, and leave for the future a detailed analysis to more realistic cases with respect to geometry and material composition, which is necessary for the physics of nuclear reactors.

2. BOLTZMANN TRANSPORT EQUATION AND THE MONTE CARLO IN THE PARTICLES TRANSPORT

The focus is put on the central problem of nuclear reactor theory, the determination of the neutron distribution in the reactor. It is the distribution of neutrons which determines the rate at which various reactions occur in the nuclear reactor core. Furthermore, studying the behavior of the neutron population will indicate the stability of the fission chain reaction cycle. In order to determine the neutron distribution in the reactor one has to investigate the process of neutron transport, i.e., the neutrons behavior in the reactor core, frequently scattered by the atomic nucleus and eventually absorbed or escaping from the reactor.

The transport theory is relatively simple, in principle, and an exact equation that governs the transport phenomena can be easily obtained. This equation is called the Boltzmann transport equation [4,7] which can be written as

$$\vec{\Omega}.\nabla\Phi(\vec{r},\vec{\Omega},E)+\Sigma_t\Phi(\vec{r},\vec{\Omega},E)=\sigma\iint f(\vec{\Omega}',E'\rightarrow\vec{\Omega},E)\Phi(\vec{r},\vec{\Omega}',E')d\vec{\Omega}'dE'+S(\vec{r},\vec{\Omega},E). \quad (1)$$

Unfortunately, it is much easier to derive the Boltzmann transport equation than to solve it.

Transport equations shall consider a variety of processes, which makes the solution of the equations a challenge. However, there is a method that allows to implement elementary processes in a stochastic form, that can be added up over the whole ensemble to characterize the full process, i.e. the Monte Carlo method [2,3,11].

The application of Monte Carlo methods for a direct simulation of particle transport phenomena is conceptually simple, one needs only to model the relevance physics of each event of the interaction of the particle, allowing the particles to propagate freely between the interactions. The implementation does not use the transport equation directly, because the particle balance between various events and the escape is simulated numerically, and all that is needed are the mathematical expressions of the probability relations for the different possible events, defined previously by the model, which then simulates the particle trajectory length until the interaction point where the event will occur. The transport equation results then as the average behavior of the whole particle population.

The essentially idea linked to the use of the Monte Carlo method is to simulate particle transport by monitoring a series of neutron histories, using random numbers to determine whether and what type of interactions occur along the path of the neutron.

3. "CONTINUOUS" PROGRAM FOR SIMULATING NEUTRON

This paper describes a stochastic model to simulate the neutrons transport in an environment composed of two distinct regions in three dimensions, as shown in Figure 1. One of the regions consists of uranium dioxide (UO_2) and the other of water. The neutron flux in this approach is seen in spectral form, it depends on energy in a continuous form.

The program considers vacuum as boundary condition on all borders of the medium, this implies that only escape is considered and there is no neutron back scattering from the external environment which contains the problem.

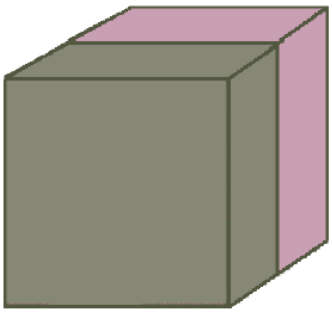

Figure 1. Environment composed of two distinct regions.

The spectrum of neutrons of the fission is the starting point for calculations in nuclear reactors. In this study, the initial energy of the neutrons is given by the spectrum of neutrons of the fission of U-235, which is approximated by the equation

$$N(E) = 1765\sqrt{E}\exp(-0.775E), \quad (2)$$

where *N(E)* is the neutron flux and *E* is the energy of the neutron in MeV [9].

The spectrum of the cross sections of the materials that constitute the medium are parametrized. Dividing the spectrum in energy ranges, for each energy range a parametrization of the cross section is determined in form of a continuous function. Fig. 2 shows the fission cross section of uranium-235 from original data, obtained from the website of the International Atomic Energy Agency (IAEA) [10], and our parametrization, the blue curve shows the real of the fission cross section spectrum of uranium and the black curve is the approximation obtained by the parametrization, where the parameters have been determined by inference with the real fission cross section data. Then, each energy range has a specific function. In principal the parametrization may be improved once a new set of data or better data are available. The inclusion of the continuous energy dependence in the solutions improves the results and will indicate, among others, how the spectral distribution influences the nuclear criticality.

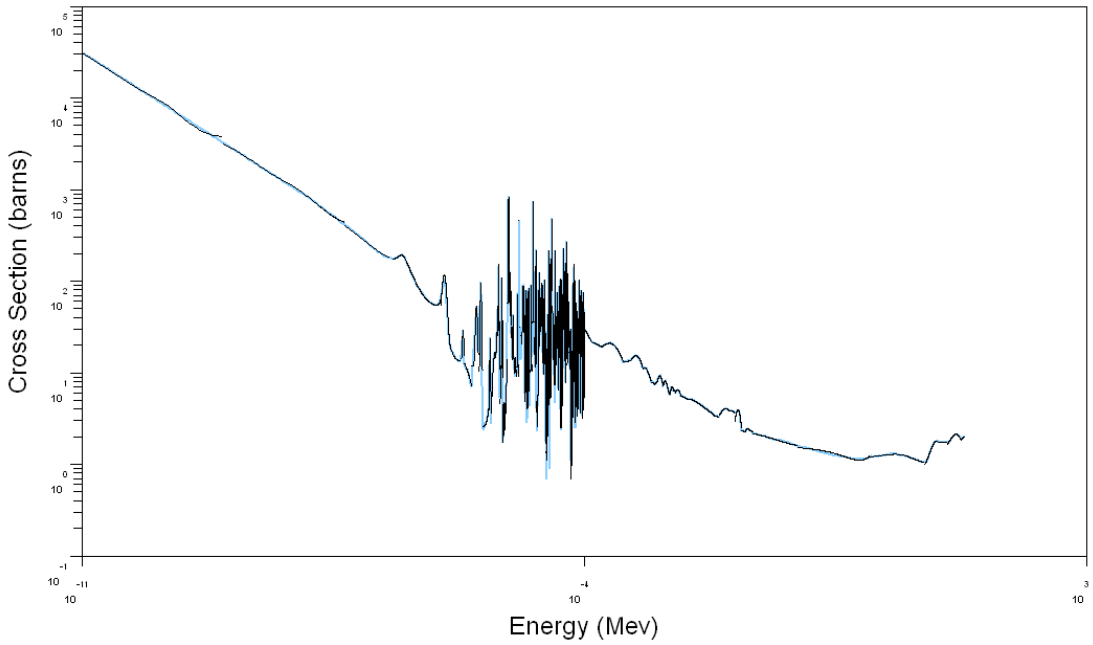

Figure 2. Parameterization of the fission cross section of the uranium-235.

For a realistic computational simulation of the flux of neutrons in a reactor is necessary to follow the life history of a large number of neutrons, compatible with fluxes of the order of $10^{13}cm^{-1}s^{-1}$ or larger. This will consume a considerable computational time, which would make the simulation long, not to mention the cost of processing and memory would be high. Due to this fact, this study divided the volume analyzed in several parts, which were called sub-volumes.

After defining the sub-volumes, call one of those sub-volumes as the volume of control in uranium dioxide and choose another to be the volume control in water. It is from these control volumes that the problem proposed is being studied. The implementation of the concept of control volume allows you to computationally simulate the behavior of a population of neutrons in a given environment by accompaniment the life histories of a number of neutrons below that required in common simulations.

A peculiarity of the program is that one can define a large number of initial neutrons, for example, 10^6, and simulate various scenarios of criticality keeping this number constant and varying the size and therefore the number of sub-volumes, i.e., the volume size of control regulates the regime of criticality in the simulation.

Once analyzed the processes occurred in the volume of control, just use a weighting to rescale the processes that could possibly occur in other sub-volumes, taking into account that in principle the physical processes are the same except for the escape probability, which depends as much on energy as the position of the volume in consideration. This weighting is estimated using an auxiliary program. In this auxiliary program weighting is computed through a relationship between the number of neutrons that escape the medium, from the sub-volumes analyzed, and the number of interactions that sub-volumes.

The program is developed in the C++ language, and received the name of “Continuous”. In program the neutron can move in all directions. During its life story the neutron may suffer three types of interactions with the medium, absorption (radioactive capture), elastic scattering or fission, but can also escape from the medium. The program is terminated when the life history of all neutrons are accompanied.

4. RESULTS ANALYSIS

First, we must emphasize that the work should be considered as a first step in a direction where the continuous energy dependence and local dependence of the neutronics are considered. Therefore this study makes use of only a small selection of materials that constitute the "core of a reactor", water and uranium dioxide, and additionally used a simple geometry, especially for validating the model implementation. In future more realistic simulations will be performed, once the method works so that the rest is just changes in the geometry of the medium and the conditions imposed on the problem.

As part of this study, we examined the density of neutrons in control volumes of fixed size and their dependence on the size of the total volume. This has the finality to verify the effects related to volume, i.e., physical interactions and to surface, i.e., escape. The influence of surface-volume ratio in the density of neutrons is shown in Fig. 3. The increase in the density of neutrons with the growth of the volume was expected, since increasing the size of the

environment approaches more and more a situation of an infinite medium, where there is less escape. It should be noted that between volumes of edges of 20 cm and 30 cm the density changes from a monotonically decreasing curve to a curve that has a maximum at a time different to the zero Monte Carlo step ($t_{MC}= 0$). This is due to the fact that by increasing the dimensions of the environment consequently increases the number of scatterings, the number of captures and the number of fissions, thus increasing the Monte Carlo instant criticality for that step, leading to the conclusion that criticality varies along the steps. The number of neutrons is computed by adding the neutrons that are born in the control volumes, including here the neutrons from fission, with neutrons that were scattered for these volumes.

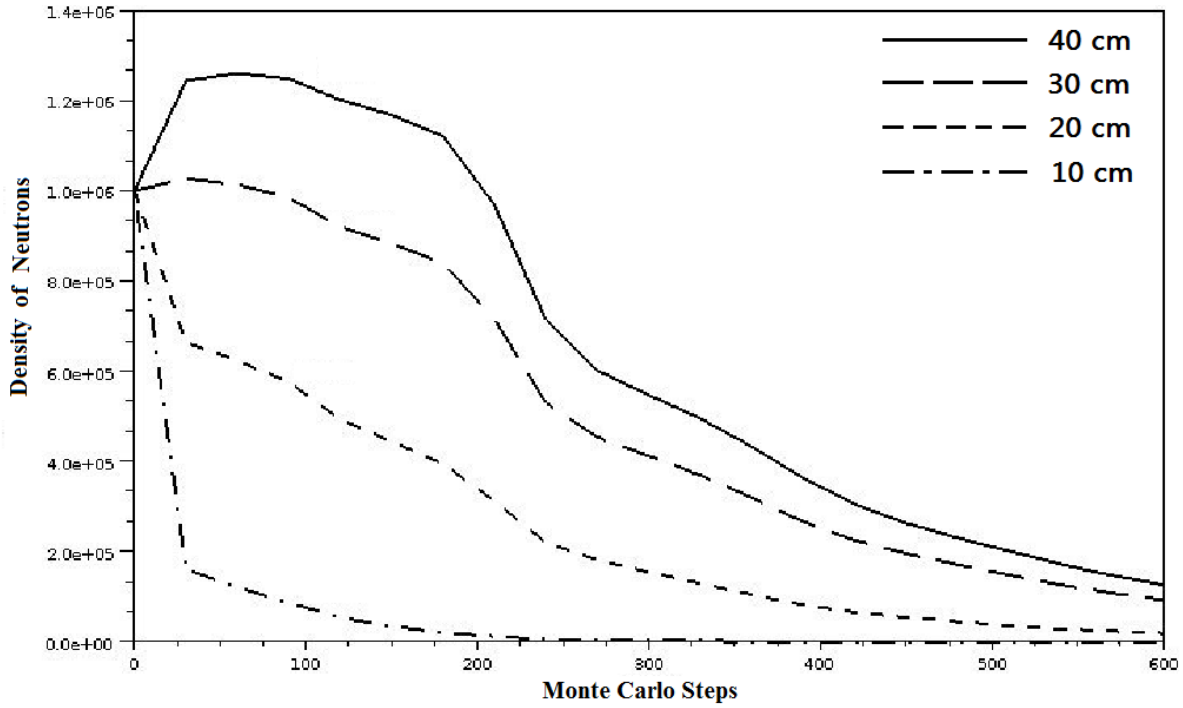

Figure 3. Neutron density over time in units of Monte Carlo steps in volume control, keeping constant the number of sub-volumes.

In order to check the density of neutrons by the size of control volumes a study was realized where the size of the edges that define the total volume was kept the same, now varying the number of volumes of control. Here we use a medium consisting of 216, 1000 and 3375 sub-volumes, respectively. Care was taken in all cases so that the sizes of the edges of control volumes were of the order of magnitude of the mean path free of neutrons in the environment. In all three analyzed cases the size of the edges that define the cubic environment are the same (30 cm) and the initial number of neutrons is 106.

The numerical results of this study are shown in Fig. 4, where we can observe that unlike the earlier study, there is no pronounced change in the curve that describes the density of neutrons in the control volume. What can be noted here is a difference in the decay intensity

of density curves along the Monte Carlo steps. During the studies we verified that increasing the size of the edges that define the environment, at a certain moment the size of the control volume may interfere in the criticality of the problem, i.e., can simulate different criticalities by simply varying the dimensions of those volumes.

We also verified that decreasing the size of the control volume does not avoid the escape from the environment, only increases the number of interactions suffered and the number of neutrons generated. The advantage of using smaller control volumes is due to the fact of getting a higher concentration of neutrons, thus offering the possibility to monitor a small number of life stories of neutrons and still resulting in an approach with acceptable fluctuations on the average behavior of neutrons in the environment, which is rescaled for all sub-volumes of the environment by weighting that corrects the density for the local escape probability depending on the position of the sub-volume in the total volume. We have chosen the density of neutrons in the verification, because this is more intuitive.

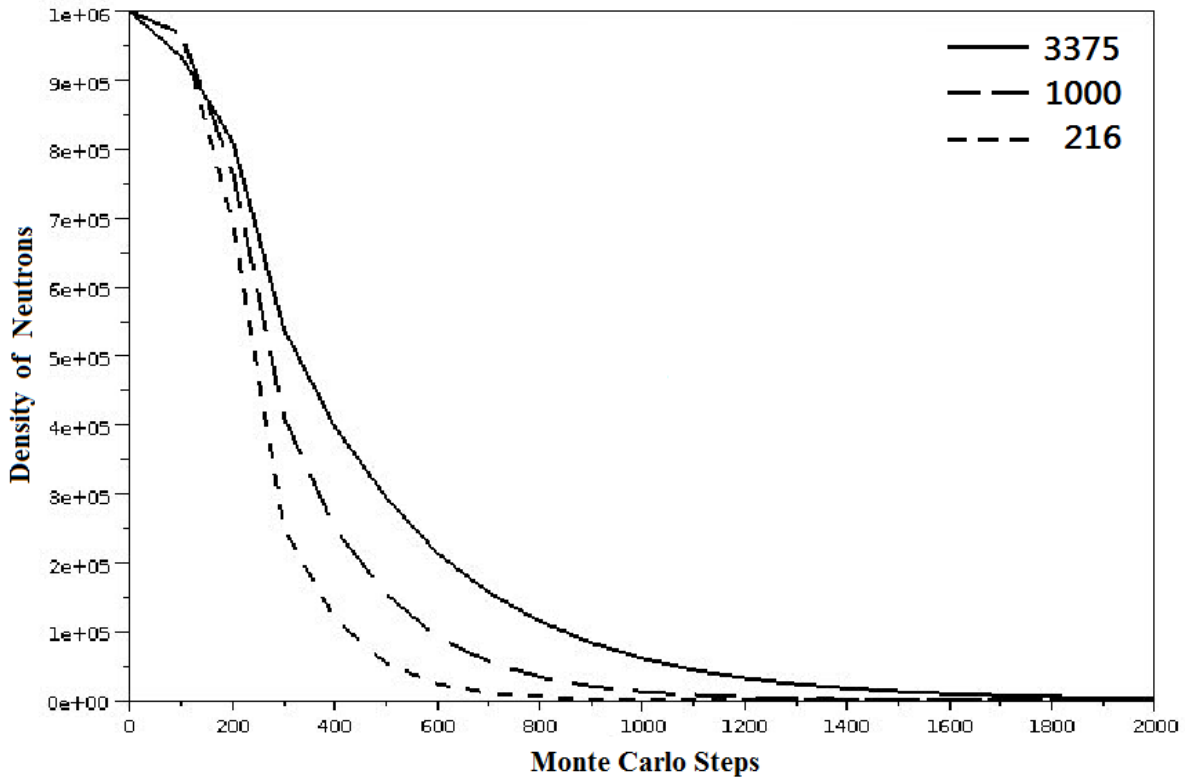

Figure 4. Neutron density over time in units of Monte Carlo steps in volume control, varying the number of sub-volumes.

Before we observed the influence of the geometry on the density of interactions and on the escape of neutrons. Now, the spectral aspect in the development of neutron populations is analysed and its temporal dependence, here in units of Monte Carlo steps. As principal quantity of the analysis we introduced a multiplication factor of the simulation that we call

here the Monte Carlo instantaneous spectral multiplication factor. At this phase of the work only spectral dependence and dependence of the size of the control volumes are investigated, there is the possibility and need to extend the procedure also for a local analysis, i.e., dependent of the position.

For this purpose we use a cube of edge equal to 80 cm and 106 sub-volumes, with 104 as the initial number of neutrons. The Monte Carlo step is a quantity that may be related to a time scale after calibration. Defined the time scale can be obtained the effective multiplication factor, k_{eff}, when the simulation reaches a steady state and the number of steps between successive generations is counted. In a simplified form we can verify this behavior. If each of the 104 initial neutron starts with Monte Carlo time $t0_{MC}=0$, then the ensemble of the neutrons that arise by fission reactions in an instant $t_{MC}> 0$ produces a peak in the temporal sequence. Of course these temporary marks dissipate from one generation to another. It should be remembered here that we did not include precursors coming from of the decay of fission products, which would change the procedure of the temporal calibration.

The peaks found in Fig. 5 identifies the generations, these peaks are attenuated along the steps due to thermalization of the neutrons when they interact in the water. The series of steps that fission neutrons realize to reduce their energy to thermal energy and to be absorbed in the reactor to produce further fission is referred as the neutron life cycle.

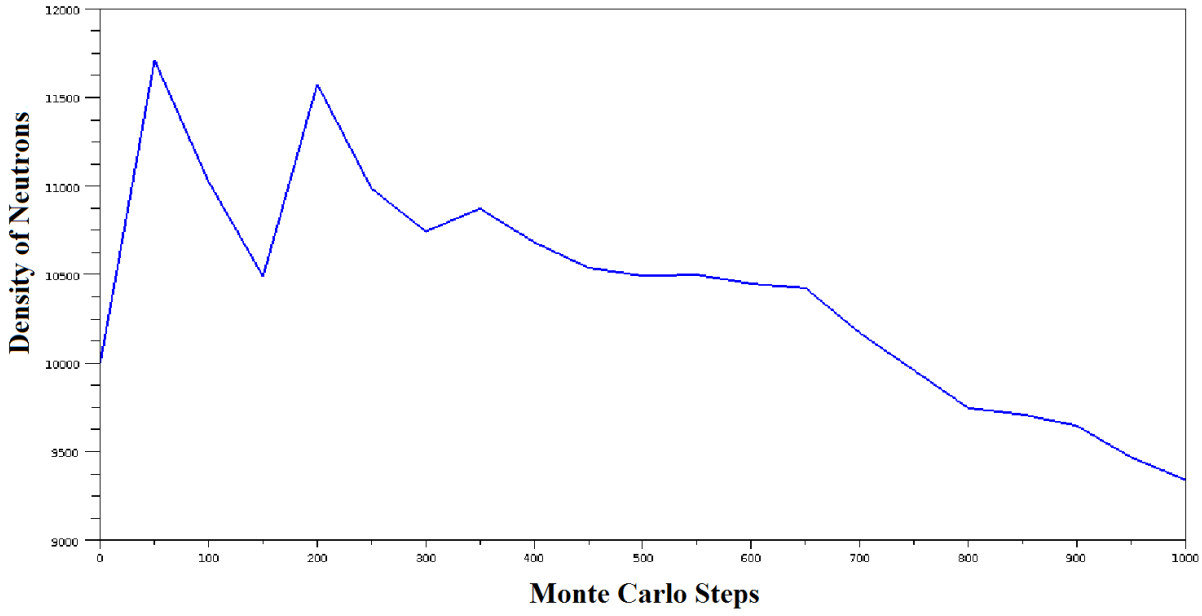

Figure 5. Identification of the life cycle of neutron and Monte Carlo steps.

In Fig. 6 is found the distribution of neutron energy for a sequence of Monte Carlo steps. There is a more pronounced change in the region of higher energies. The more energetic neutrons are, coming from fission, which justifies that this change is more pronounced in the

energy spectrum of neutrons in the range of higher energies. After neutrons being scattered causes a drop in neutron energy than the original neutrons number in this range, i.e., the spectrum of neutrons suffers a significant change over time. The Fig. 7 gives the change in the spectral multiplication factor with the Monte Carlo steps. What is observed here is a significant dependence of energy between the spectral density of neutrons for a given time step Monte Carlo in comparison its density in the previous step.

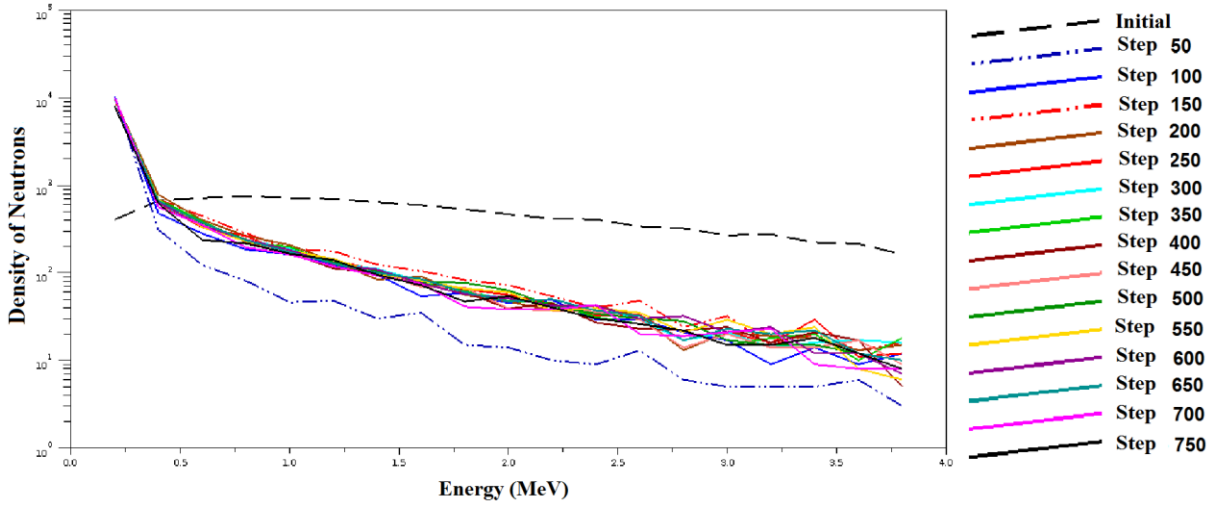

Figure 6. Energy distribution along the Monte Carlo steps.

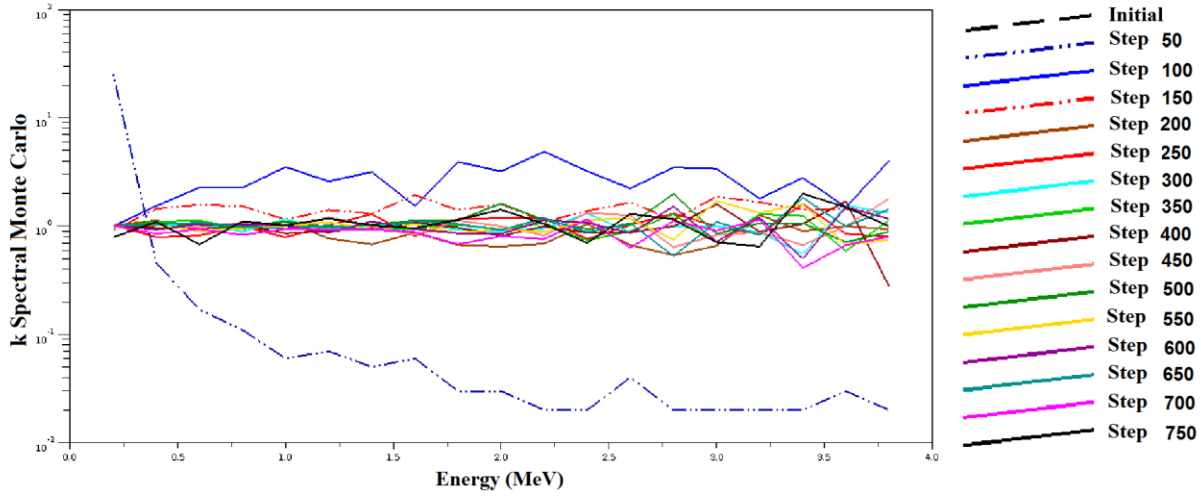

Figure 7. k spectral Monte Carlo along the steps.

4. CONCLUSIONS

We are aware of the fact that the problem approached in this work is far from being comparable to a nuclear reactor, but in this discussion the main target was to develop the Monte Carlo model for the neutron transport, implement the code in a computational language that allows extensions in modular fashion, and evaluate the internal consistency of this code to ensure the fidelity in the results when complex arrangements are used. It should be noted that the only module that needs to be changed is that which contains the three-dimensional geometry of interest. The modules that control the criticality, the propagation of the neutrons and the interactions were evaluated and considered as satisfactory. Differently to many approaches in the literature, we considered here a three-dimensional geometry and the continuous dependence of energy instead of the usual energy groups. For this purpose, functions with the cross sections in parameterized and analytical form were provided. This allows a detailed analysis of the influence of energy on the neutron population and its impact on the life cycle of neutrons. With these new results we observed the changes in the energy spectrum of neutrons with steps of simulation. From the results, even for a simple geometrical arrangement, we can conclude there is need to consider the energy dependence, i.e., an effective spectral multiplication factor should be introduced for each energy group separately. The use of a single k_{eff} means independence of the spectrum of neutrons for their reproduction. However, from the simulation arises that in case of (pseudo-)stationariety the spectrum can be constant on average over a large enough time interval. There are discussions in the literature that analyze the fluctuations in the spectrum of neutrons that confirms the existence of a recursively mode as reported in reference [1]. In this state of the developments the precursors were not included. The presence of delayed neutrons is especially important when it comes to the question of the effective lifetime of the neutrons, a quantity relevant to calibrate the unit Monte Carlo step in units of time such as seconds. Additionally we intend to develop a future work also quantities like scalar flux, reaction rate, local escape and its energy dependence, and rate of local moderation with its specific energy spectrums. We also have interest to enrich the "Continuous" program, making possible other types of neutron interactions during their path in the environment, for example, the inelastic scattering and up-scattering. Future results are expected to obtain data to establish analytical functions of the respective distributions, which in turn can be used in analytical approaches, semi-analytical or hybrid models. In conclusion, we can say that, having presented the results that prove the well functioning of the model, open up for possibilities for a variety of analysis, which can contribute to learn and understand the details of the neutronics relevant to the understanding of nuclear reactors neutrons or to the development of new concepts for reactors.

ACKNOWLEDGMENTS

This paper was supported by Comissão Nacional de Energia Nuclear (CNEN).

REFERENCES

1. C. S. Gil, “Generation of the Continuous Energy Cross Section Data for the MNCP Code”, *Nuclear Data Evaluation laboratory*, Korea Atomic Energy Research Institute, Yousong-gu, Daejon, Korea (2001).

2. E. E. Lewis, W. F. Miller, *Computational Methods of Neutron Transport*, John Wiley & Sons, New York (1984).
3. F. B. Brown, *Fundamentals of the Monte Carlo Particle Transport*, Lecture notes for Monte Carlo course, Los Alamos National Laboratory, California, U. S. A. (2005).
4. G. I. Bell, S. Glasstone, *Nuclear Reactor Theory*, Van Nostrand Reinhold Company, New York (1970).
5. H. Sekimoto, *Nuclear Reactor Theory*, COE-INES, Tokyo Institute of Technology (2007).
6. J. J. Duderstandt, L. J. Hamiltton, *Nuclear Reactor Theory*, John Wiley & Sons, New York (1976).
7. J. J. Duderstadt, W. R. Martin, *Transport Theory*, John Wiley & Sons, New York (1979).
8. J. Spainer, S. Gelbard, *Monte Carlo Principles and Neutron Transport Problems*, Addison-Wesley (1969).
9. L. Cramberg, G. Frye, N. Nereson, L. Rosen, "Fission Neutron Spectrum of U^{235}",*Physical Review*, Vol. 103, pp. 662-670 (1956).
10. "Nuclear Data Services", http://www-nds.ipen.br (2010).
11. W. K. Matthes, "Monte Carlo Simulation of Neutron Transport in Intense Neutron Fields", *Annals of Nuclear Energy*, Vol. 35, Issue 12, pp. 2436-2439 (2008).