CRITICALITY ANALYSES BASED ON THE COUPLED NJOY/AMPX-II/TORT SYSTEMS

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ABSTRACT

The TORT computer code, a S_n 3-D transport program is employed for the analyses of two experiments performed at the IPEN/MB-01 reactor. The analyses reveal that TORT is very sensitive to the number of both fine and broad groups as well as to the number of up-scattering. The traditional four group structure extensively used in reactor analyses can not be used for the TORT K_{eff} calculations. The results are unacceptably high. Compared to MCNP-4B K_{eff} results, TORT and its cross section generation path have a tendency to overestimate both the fuel and control bank reactivities. The analyses show that for the critical control bank position the tendency has been to cancel both effects and the very good agreement between TORT and MCNP-4B is simply fortuitous. TORT requires practically the same CPU time of MCNP-4B for the same problem condition. If the analyses require only the K_{eff} results, MCNP-4B is more adequate than TORT due to its better mathematical and geometric description of the problem. On the other hand, TORT can be considered a valuable tool to calculate mainly localized effects such as the fission density distribution in heterogeneous core. The MCNP-4B results are very unstable and the CITATION values are underestimated at the core-reflector interface. Finally, the procedure to generate the TORT cross section library has to be subject to a great deal of research yet if this program is to become a benchmark tool.

I - Introduction

The reactor physics area has been considerably benefited from the recent progress in the calculational scheme. At the same time, the availability of faster and faster computer systems has made possible to design several sophisticated computer codes for a wide variety of applications Even for the developing country point of view the restrictions to acquire modern computer hardware has drastically reduced and most of recent advances can be of prompt availability. Recent progress in the mathematical and computational techniques for the nuclear reactor analyses has created new opportunities for research. Regarding the development of deterministic approaches, the computer code TORT[1] (Three Dimensional S_n Code) was developed at Oak Ridge National Laboratory and it is available to the nuclear community through RSICC. The TORT computer code provides a great opportunity to the reactor physicists in their tasks to simulate several three-dimensional systems in a great deal of applications. For instance, the diffusion codes have been the main tool of reactor analyses for several years. Therefore with the advent and prompt availability of modern and faster and faster digital computers, the TORT computer code can provide the reactor physicist in general with an opportunity to make 3-D analyses based in a deterministic approach of the solution of the neutron transport equation. Aiming to contribute to the code application and to some extent to the code validation, the purpose of this work is to show the methodology applied in the criticality analyses of the zero power IPEN/MB-01 reactor. Two distinct situations will be considered: the critical mass configuration and the critical state considering the 28x26 configuration with the control rods at 58.5 % withdrawn position. For the second case, it will also be considered a comparison of the relative fission density obtained from the fuel rod gamma scanning technique. The IPEN/MB-01 reactor possesses a very compact and heterogeneous core and the experiments selected will be a very hard test for TORT and the procedure to generate its cross section library. The TORT results will be also compared to those obtained using MCNP-4B[2] and CITATION[3] for the same experiments. The NJOY 94.61[4] is employed for the cross section library generation in the standard way.

II - Reactor Description

The IPEN/MB-01 critical facility is the first Brazilian zero power reactor. It consists basically a array of slightly enriched $U(4.3\ wt\%)O_2$ fuel rods immersed in a light water moderated (non-pressurized) tank. Criticality is reached by means of control rod (Ag-In-Cd) motion. The reactor was conceived to be a very flexible core to allow several basic reactor physics experiments to be performed, and also some sort of shielding experiments. Since its first criticality several experiments were carried out: critical mass, spectral indices, in-core flux mapping, gamma scanning, temperature reactivity coefficients, burnable poison, control rod calibration, noise analysis, etc. Therefore, IPEN/MB-01 reactor is used for the validation of computational methodologies and related cross section libraries, and furthermore it is also used for training and teaching graduate students and reactor operators. The complete description of the IPEN/MB-01 reactor can be found in Refs.5 and 6.

III -Experiment Description

Two experiments performed at the IPEN/MB-01 reactor were considered for the TORT analyses. Both experiments are considered at room temperatures (293 K). The first one is the critical mass configuration, which was obtained during the approach to critical experiment in the first criticality of IPEN/MB-01 reactor. The critical configuration is shown in Figure 1. The criticality was reached with a total of 564 $\pm$ 2 fuel rods. In this case the safety and the control banks are completely withdrawn and there are no need to consider them in the TORT analyses.

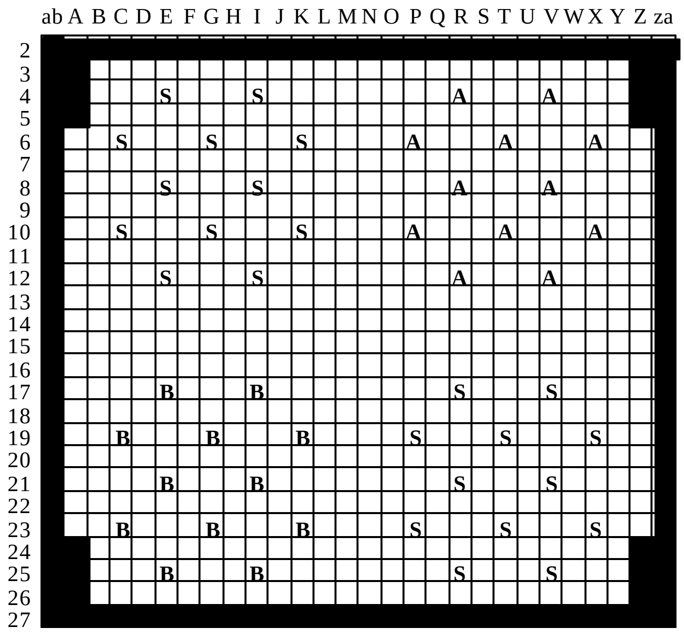

Figure 1. Cross Sectional View of IPEN/MB-01 Reactor Core for Critical Loading.

The second experiment considers the 28x26 fuel rod configuration as shown in Figure 2. The notation **S** stands for safety banks and **A** and **B** for control banks. In this case the safety banks are completely withdrawn and the criticality is reached by positioning properly the control banks. The criticality was reached when both of the control banks are at 58.5 % withdrawn position. The reference level is the bottom of the active core. The relative fission density distribution in the active core of the reactor was also of concern for the TORT analyses. This experimental quantity was obtained through a fuel rod gamma scanning technique considering the total counting of the fission product gamma emission above 600 keV. The relative fission density distribution was measured in a great deal of details. The experimental apparatus was conceived to have a collimator size of 1cm. All gamma emission above 600 keV was counted in a NaI detector. The proportionality between total gamma counting and fuel rod fission density was demonstrated in a great deal of details. Therefore, starting from the bottom of the fuel rod active length every other 1cm of fuel rod active length was considered to get the total gamma emission and consequently the relative fission density distribution. Several positions were subject to the fission density measurements but just a few of them were chosen for the TORT analyses.

The uncertainties assigned to the experimental values used in this work are 40 pcm for the critical mass experiment (the value of two fuel rods), 1 pcm for the critical control bank position. As shown extensively in Ref. 5, the control bank position indicator of the IPEN/MB-01 reactor is a very accurate system and consequently the uncertainty on the control bank position is very small. The relative fission density has a maximum uncertainty of 0.006. Consequently, the experimental data have the desired quality for a benchmark problem.

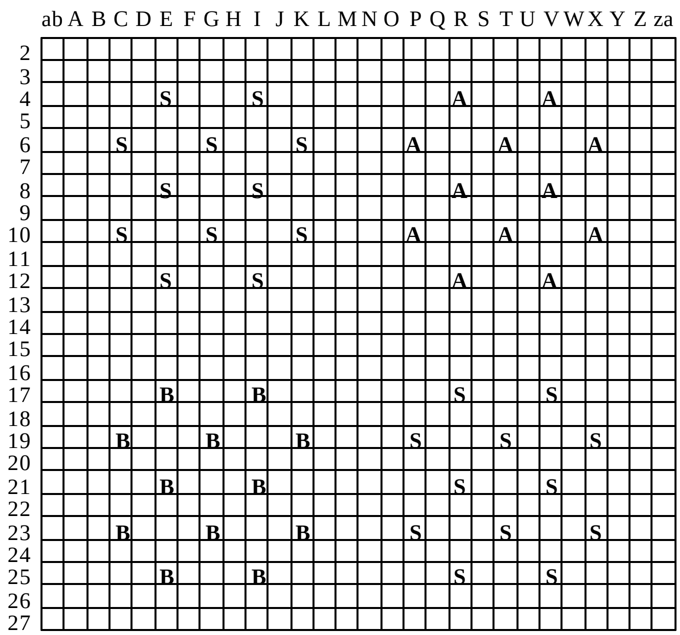

Figure 2. Cross Sectional View of IPEN/MB-01 Reactor Core.

III - Calculational Methodology

The calculational methodology applied for the deterministic calculations is shown in Figure 3. Basically, starting from ENDF/B-IV[7], ENDF/B-V[8] and JENDL-2[9] nuclear data libraries, the well know NJOY system (version 94.61) was employed to access and to process these nuclear data file in a fine group structure. The analyses of the critical experiments considered the following nuclear data: ^{238}U from JENDL-2, ^{107}Ag, ^{109}Ag, ^{115}In and ^{113}In from ENDF/B-V and the remainder of the data from ENDF/B-IV. The thermal scattering law for hydrogen bound in water was taken from ENDF/B-III[10]. Most of the analyses were based in these nuclear data sets. At the end, ENDF/B-VI release 5[14] was also considered in the analyses using the most appropriate group structure and S_n order.

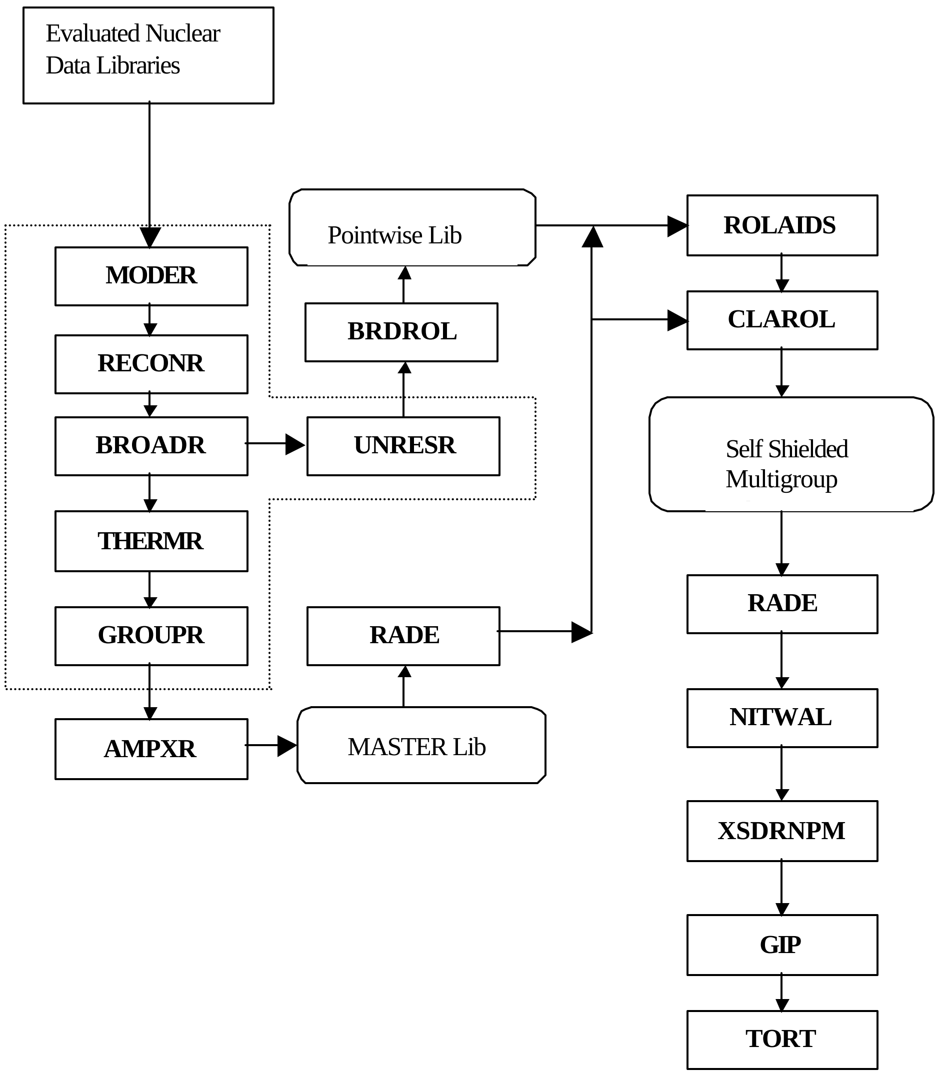

Figure 3. Schematic Diagram for the Deterministic Calculational Methodology

The RECONR, BROADR, UNRESR, THERMR and GROUPR modules of NJOY are used in order to reconstruct and to Doppler broaden the cross sections, to calculate the self-shielding effects in the unresolved resonance region, to build the scattering matrices in the thermal region, and to transform these data into multigroup parameters, respectively. The next step was the production of set of broad group energy library using the AMPX-II[11] package. The pointwise and fine multigroup cross sections produced in the previous step are transferred to AMPX-II by two in house interface modules AMPXR and BRDROL. The self-shielding treatment of the actinide resolved resonances in the neutron energy region from 0.625 eV to 5.53 keV was carried out by ROLAIDS and the neutron spectra in the several regions of the

IPEN/MB-01 reactor by XSDRNPM. Firstly, XSDRNPM considered an infinite array of fuel pin cells. The K_{inf} spectral calculations were performed in the fine group structure considering a white boundary condition at the outer boundary of the cylindrized cell. The cross sections are homogenized in a fine group level. Next, these data are merged with those of another regions such as radial, top and bottom reflectors and so on. Finally, XSDRNPM considers radial and axial slices of the IPEN/MB-01 reactor to get the final spectra for the broad group collapsing. The broad group cross sections of the control rods, guided tube, and bottom plugs were obtained using a super-cell model. At this point, the cross section library is problem dependent. Two sets of fine multigroup structure were considered to generate the broad group library: 85 groups and 620 groups (SAND-II structure). These two sets of fine multigroup were collapsed to several different numbers of broad groups: 4, 10, 14, 15 and 16 with different number of upscattering. The order of scattering (Legendre order expansion) was P_3 throughout the analyses. Finally, the broad group library is conveniently formatted to the TORT (3D Discrete Ordinates Code) format using the GIP[12] program. Subsequently, using the cross sections libraries generated before, TORT performed K_{eff} and reaction rate calculations considering a fully tri-dimensional geometric modeling of the IPEN/MB-01 reactor core.

The calculational methodology applied for the stochastic calculations is shown in Figure 4. The basic nuclear data are accessed and processed by the NJOY code, which reconstruct, broadens, and formats the data into the appropriate form for MCNP-4B using the ACER module. The MCNP-4B library was constructed consistently with the same nuclides and nuclear data files as used in the deterministic approach. The RECONR and BROADR modules of NJOY were run with 0.5% and 0.2% interpolation tolerance respectively for all nuclides. The thermal neutron scattering files $S(a,b)$ needed for hydrogen bound in water were obtained with LEAPR module of NJOY.

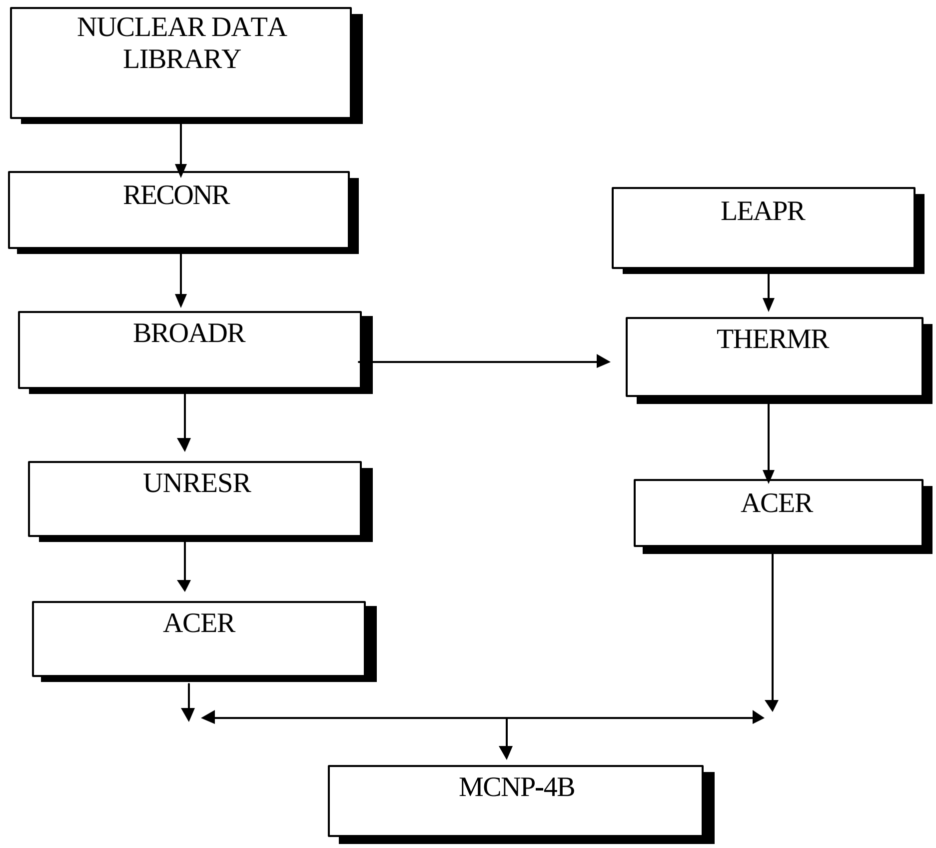

Figure 4. Schematic Diagram for the Stochastic Calculational Methodology

IV - Calculational Model

Deterministic. The fully three dimensional geometric setup for the TORT calculations was considered with the X-Y-Z geometry, P_3 approximation, angular quadrature from S_4 up to S_{16}, and a variable number of groups as well as thermal upscattering. The mesh distribution comprises 52 mesh intervals in X direction, 50 mesh intervals in Y direction, 81 mesh intervals in Z direction, for a total of 210600 intervals. These intervals are represented by 10 numbers of material zones. The boundary conditions considered were void at top and bottom and at the left and right borders of the problem. The convergence criterion for the criticality calculations was set to the 5.000E-04 for the flux and 1.00E-05 for the eigenvalue. The total axial fission reaction rate was obtained using the converged flux. The CITATION modeling of the IPEN/MB-01 core was performed consistently with the TORT approach. In this case the whole cross-section set was prepared by HAMMER-TECHNION[13]. The nuclear data used in the analyses are again consistent with those used by TORT.

Stochastic. The MCNP-4B geometric modeling of IPEN/MB-01 reactor core was considered in a very high level of details to give a nearly exact description of the reactor system. The criticality calculations were made considering a very high number of neutron histories. It was considered 500 batches of 10000 neutron histories each which gives a total of 5 millions neutron histories. The fission rates were calculated considering 40 millions of neutron histories in order to achieve a standard deviation of around 3%. In this case, the geometric modeling considered the division of the fuel rod in several axial plans in order to get the fission rate distribution consistently with the positions and volume of the measurements.

V - Results and Discussions

Even though the quality of TORT results can not be dissociated to the quality of the nuclear data and their processing path, several considerations can be drawn readily to the TORT performance in the analysis of the experiments of this work. In this sense, the main emphasis of the discussions will be employed to the calculational characteristics of both the cross section generation path and the three-dimensional neutron transport path. This aspect is important because to have TORT useful for a benchmark tool the whole calculational uncertainties have to be minimized.

V.1 - Criticality Calculations

Consider initially the TORT analyses of the 28x26 fuel rod configuration as shown in Figure 2. Table I shows the TORT K_{eff} results along with the MCNP-4B and CITATION results. The first aspect to be noted in Table I is the very high sensitivity of the TORT K_{eff} results to the number of both fine and broad groups, and mainly to the number of up-scattering groups.

Table I. - K_{eff} results for the 28X26 critical configuration.

Case	Energy Group Structure Fine/Macro	Legendre Order Expansion	S_n Quadrature Order	Number of upscattering	K_{eff}
1	85/4	P_3	4	0	1.02044
2	85/10	P_3	10	1	1.01251
3	85/14	P_3	10	4	1.01011
4	85/15	P_3	10	5	1.00997
5	620/16	P_3	10	5	1.00563
6[a]	620/16	P_3	10	5	1.03214
CITATION	-	-	-	-	1.00142
MCNP-4B	-	-	-	-	1.00585± 0.0002

a - control banks fully withdrawn

The four group structure shown in Table I is the traditional one with breakpoints (10 MeV, 0.8205 MeV, 5.53 keV, 0.625 eV, and 1.00E-05 eV) extensively used in several reactor physics applications. From the data shown in Table I, it can be seen clearly that TORT can not be used in conjunction with such small number of broad groups. The K_{eff} results are unacceptably high. Comparing cases 2 and 3, it can be noted an improvement of around 240 pcm, simply by increasing the number of thermal groups and consequently the number of up-scattering. However, a small effect was observed in cases 3 and 4 where the number of thermal groups was increased by one group. The tendency has been to saturate. The biggest change was observed when the number of fine groups was increased to 620 groups (SAND-II structure). In this case, it was observed an improvement of 434 pcm relative to case 4. In this case, the K_{eff} calculated by TORT is very close to the one obtained by MCNP-4B. The CITATION result is the Closest to the experimental value but the analyses of this achievement is very difficult. From the mathematical point of view, MCNP-4B can be considered a reference. Therefore, in the CITATION case, it may be occuring some sort of compensating errors.

Table II shows the TORT K_{eff} sensitivity to the quadrature order. In this case, the study has been restricted to case (620/16); i.e., the fine group spectra calculations performed with 620 groups and the TORT broad group analyses with 16 groups. Table II shows that the maximum difference observed is around 170 pcm. The largest relative difference was observed for S_4 (case 7). However this case shows a poor angular discretization because it contains just two angles. The K_{eff} behavior against quadrature order is not asymptotic. The reason for that was not found during the execution of this work. It can be due to several reasons including the procedures to generate the quadrature set, numerical accuracy of the computer employed and so forth.

Table II. K_{eff} results for the 28x26 critical configuration against Sn order.

Case Number	Energy Group Structure Fine/Macro	Legendre Order Expansion	S_n Quadrature Order	Number of upscattering	K_{eff}
7	620/16	P_3	4	5	1.00416
8	620/16	P_3	6	5	1.00520
9	620/16	P_3	8	5	1.00526
10	620/16	P_3	10	5	1.00563
11	620/16	P_3	12	5	1.00488
12	620/16	P_3	14	5	1.00589
13	620/16	P_3	16	5	1.00506
MCNP-4B	-	-	-	-	1.00585± 0.0002

Table III shows the TORT K_{eff} results for the critical loading configuration shown in Figure 1. Here, it is only considered the case (620/16) which can be considered the best fine and broad group structure for TORT. Also shown in Table III are the HAMMER-TECHNION/CITATION and MCNP-4B results. The mismatching of the K_{eff} results is very noticeable but the explanation is very difficult due to the distinct approaches adopted by the three methodologies. The agreement between TORT and MCNP-4B in this case is not as good as in the previous case (see Table I). TORT overpredict the K_{eff} relative to MCNP-4B by an amount of around 382 pcm. In the previous cases the agreement was inside 70 pcm. Consequently, there has been left a suggestion that there is an overprediction of the control bank worth. In order to show that , case 6 of Table I shows the K_{eff} when all control rods are completely withdrawn. The reactivity excess calculated by TORT is 3214 pcm. On the other hand, the experimental reactivity excess inferred from the control bank worth is 2415 ±84.5 pcm. There is a difference of 799 pcm between theory and experiment. This difference is much bigger than the reactivity excess experimental uncertainty and therefore can be credited totally to the calculational methodology and related cross section library.

Table III. K_{eff} results for the Critical Loading Configuration

Code	Energy Group Structure Fine/Macro	Legendre Order Expansion	Quadrature Sets	Number of upscattering	K_{eff}
TORT	620/16	P_3	10	5	1.00795
CITATION	----	----	--	0	1.00180
MCNP-4B	----	----	--	----	1.00413 ± 0.00030

Now, turning attention to the critical mass experiment (Table III), there is a reactivity difference of around 795 pcm between the TORT predicted value and the experimental value (K_{eff} =1.00). Again here, the difference is much bigger than the experimental uncertainty (40 pcm) and can be credited totally to the calculational methodology and related cross section library. This reactivity difference is consistent with the difference on the reactivity excess found in the 28x26 configuration. It means that the K_{eff} bias found for the fuel and reflector regions in the critical mass experiment is preserved on the 28X26 configuration. Therefore taking for example case 5 of Table I there is a K_{eff} overprediction of 536 pcm. Out of this value, 799 pcm is due to the fuel and reflector regions and –263 pcm is due to the control banks. Consequently, the anti-reactivity of the control banks is overestimated by 263 pcm. The MCNP-4B is nearly an exact solution for the neutron transport problem of the IPEN/MB-01 reactor. The very good agreement between TORT and MCNP-4B K_{eff} results shown in Tables I and II is simply fortuitous.

Table IV shows the K_{eff} results considering the last release of ENDF/B-VI (release 5). In terms of eigenvalue quality there is a very good improvement compared to the libraries used in this work. The K_{eff} tendency found before is maintained with ENDF/B-VI release 5. Now, TORT overestimates the control bank worth by 200 pcm.

Table IV. K_{eff} Results for the Critical Configurations With ENDF/B-VI.5

Code	Energy Group Structure Fine/Macro	Legendre Order Expansion	Quadrature Sets	Number of upscattering	K_{eff}
TORT[a]	620/16	P_3	10	5	1.00458
TORT[b]	620/16	P_3	16	5	1.00249
MCNP-4B[a]	----	----	--	-	1.00230± 0.00023
MCNP-4B[b]	----	----	--	----	1.00393± 0.00010

a- Critical Mass Configuration
b - 28x26 Critical Configuration

V.2 Axial Fission Density Profiles

Just to illustrate the ability of TORT to predict the relative fission density profile in the IPEN/MB-01 core, consider positions M15, M27, ab27, and B24 (see Figure 2) which represents several extreme cases. M15 is a central position, M27 is a position in the core-reflector interface, ab27 is at the corner, and B24 is very close to the control bank. Figures 5, 6, 7, and 8 show the comparison between theory and experiment and also the MCNP-4B and CITATION results. All data are normalized to the central position of the active core. The MCNP-4B results in general are very unstable due to both the lack of convergence and its statistical nature. Particularly in this case, it was considered 40 millions neutron histories to get a standard deviation of around 3%. As expected, in the central region (position M15, Figure 5) the agreement between theory and experiment for all methodologies is very good. However the same can not be said for positions at the core-reflector interfaces (M27 and ab27) and close to the control banks (B24). The corresponding results are shown in Figures 6, 7 and 8 respectively. For the positions close to the control banks (B24), TORT underestimates the relative power distribution mainly in the upper part of the fuel rod. This effect is mostly due to the over-prediction of the control bank worth as founded previously. The CITATION and MCNP-4B results for position B24 show better agreement even considering the positions close to the core border. Considering positions M27 and ab27; the ones at the radial reflector interface, the weakness of the diffusion calculations is very pronounced. On the other hand, TORT and MCNP-4B shows a good performance but in the specific case of TORT the under-prediction of the relative power distribution at the upper part of the fuel rod is still present.

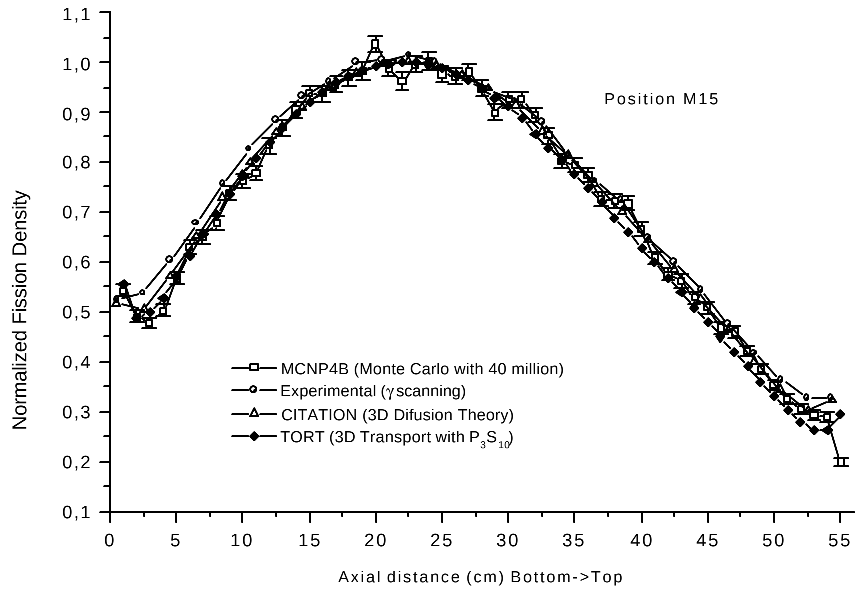

Figure 5. Axial Fission Density Profile at Position M15

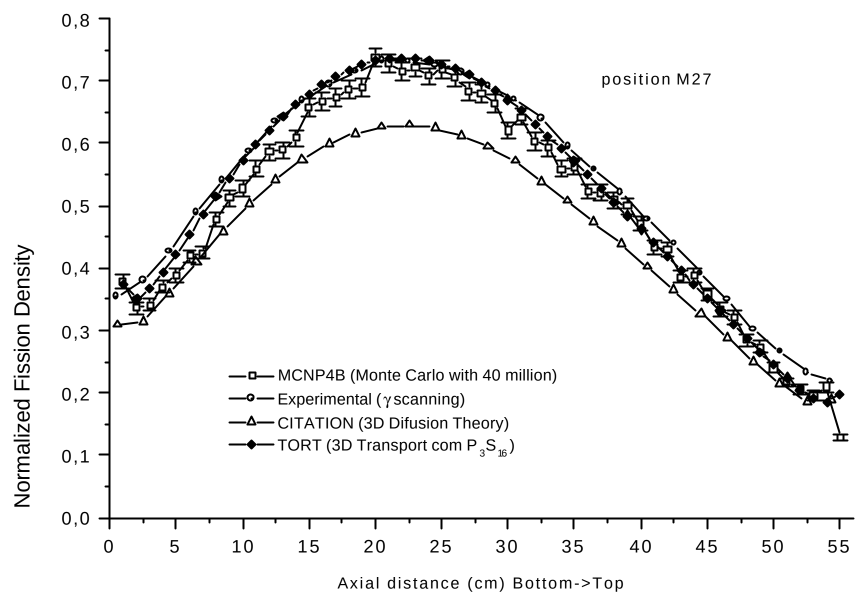

Figure 6. Axial Fission Density Profile at Position M27

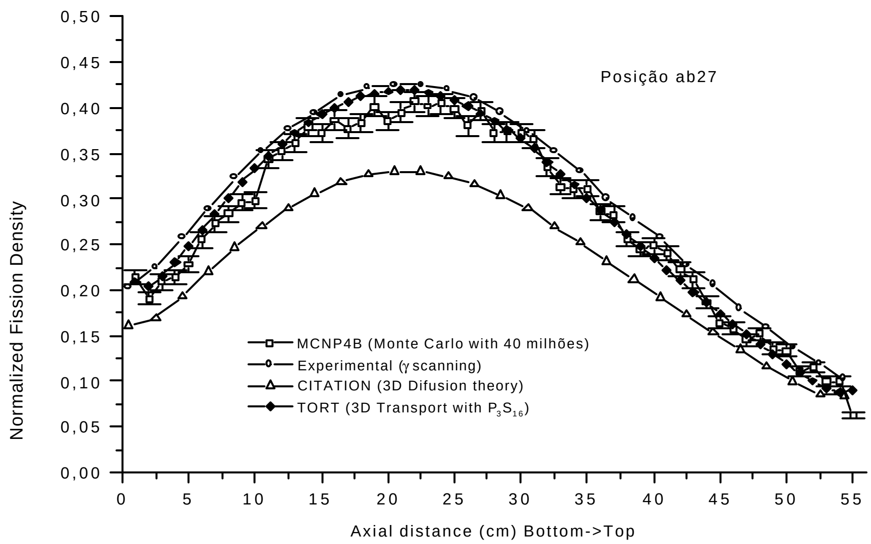

Figure 7. Axial Fission Density Profile at Position ab27

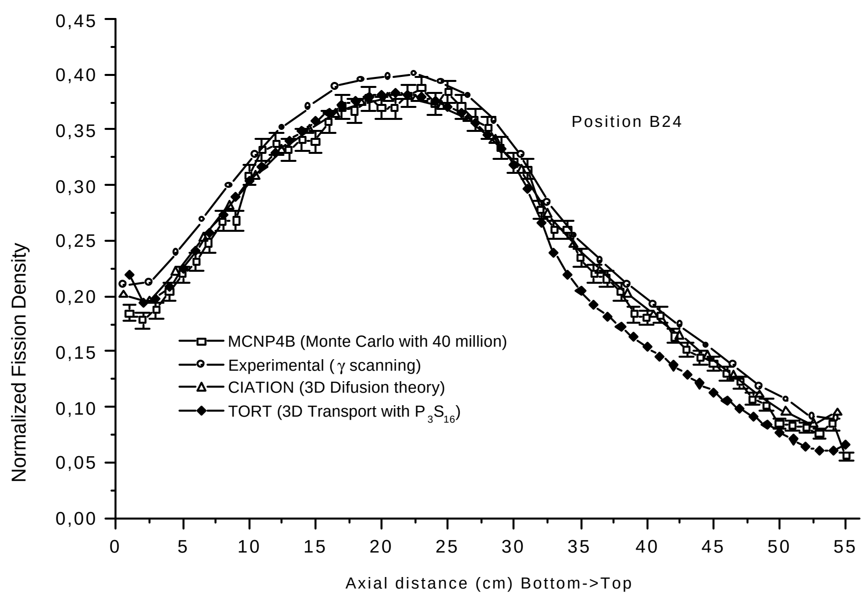

Figure 8. Axial Fission Density Profile at Position B24

VI - CONCLUSIONS

In conclusion, this work presents a calculational methodology to perform a criticality calculation using the coupled NJOY, AMPX-II and TORT systems. Two experiments performed at the IPEN/MB-01 reactor were considered in the analyses. The experimental quantities were critical configurations and the relative fission density distribution for the 28X26 fuel rod configuration. The TORT results were also compared to those of MCNP-4B and CITATION. In spite of the whole K_{eff} discrepancies are credited to both the cross section quality and its generation path and the 3-D neutron transport path, several conclusions can be drawn relative to TORT performance readily. The analyses reveal that the K_{eff} results produced by the TORT computer code are very sensitive to the number of both fine and broad groups and mainly to the number of upscaterring. The traditional four group structure as extensively used in conjunction with several diffusion codes can not be used for the TORT K_{eff} analyses. The results are simply unacceptably high. The TORT K_{eff} analyses also shows some sensitivity to the quadrature order. The largest relative difference was found with S_4. However, this quadrature order provides a poor description of the neutron directions and consequently its angular descriptions gives rise to a rather poor K_{eff} results. Compared to MCNP-4B K_{eff} results, TORT and its cross section generation path have the tendency to overestimate both the fuel and the control bank reactivities. The analyses show that for the critical control bank position the tendency has been to cancel both effects and the very good agreement found between TORT and MCNP-4B is simply fortuitous. The analyses of the axial power density profiles has to be made in conjunction with the quality of the cross sections and their generation path. However, apart from the positions close to the control banks, TORT shows a good agreement with the experimental points. Also at positions close to the radial border, TORT results are further superior to those of CITATION. Consequently, TORT can offer an alternative and precise way to calculate the fission density distribution in heterogeneous systems. Historically, such calculations have being performed by codes based on diffusion theory. Typical applications of interest could be the axial power density in BWR systems.

Finally, TORT computer code can be considered a valuable tool to calculate mainly the power density distribution in heterogeneous core but the procedure to produce its cross section library has to be subject to a great deal of research yet. In terms of CPU time, TORT is very close to MCNP-4B conditions. Therefore, TORT can be considered very useful if the calculations require localized effects such as the power density distribution. If the analyses require only K_{eff} determination, MCNP-4B is more recommended than TORT, simply because TORT require a very troublesome way of cross section generation and the CPU spent by this program is comparable to MCNP-4B. On the other hand, for this application MCNP-4B gives better K_{eff} results due to its better mathematical and geometric description of the problem.

VI - ACKNOWLEDGEMENTS

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