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THEORETICAL ANALYSIS OF THE INVERSION POINT OF THE ISOTHERMAL REACTIVITY COEFFICIENT OF THE IPEN/MB-01 REACTOR

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ABSTRACT

TORT, a S_N 3-D transport code, is employed for the analysis of the inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor. The analyses are performed in a companion NJOY, AMPX-II and TORT systems. The nuclear data library considered in this work is the last release of the ENDF/B-VI, namely release 8. The analyses reveal that for this peculiar problem there is a need to convert all the computer codes do DOUBLE-PRECISION as well as to increase the number of digits of the ANISN library generated by XSDRNPM to 7. Beyond that the number of energies for the secondary neutrons emerging in a scattering process in the thermal neutron energy region in the THERMR module of NJOY was increased to 948. The calculated inversion point is 10.53°C while the experimental one is 14.99 ± 0.15°C. At first sight it would appear to have a significant discrepancy. However in terms of reactivity coefficient this discrepancy means a deviation of -0.89 ± 0.05 pcm/°C which indicates that the calculated reactivity coefficient meets the desired accuracy (-1.0 pcm/°C).

Key Words: reactivity coefficient, TORT, ^{235}U nuclear data, IPEN/MB-01 reactor, benchmark.

1. INTRODUCTION

The isothermal reactivity coefficient has an important bearing on passive safety and inherent stability of nuclear reactors, and its better knowledge can contribute to reduce the uncertainty margins of power rise and predicted accident consequences of LWRs. Recent progress in the ^{235}U nuclear data [1, 2, 3] has culminated in new evaluated files that improved considerably the agreement between theory and experiment [4, 5, 6] of such integral reactor response for systems fueled with slightly enriched uranium. Several studies [5, 7] made with the IPEN/MB-01 core configuration suggest a very high sensitivity of the isothermal reactivity coefficient of this system to the shape as well as to the magnitude of the thermal ^{235}U cross sections. This facility has a lot of features that favor the neutron thermal energy region, and several calculated responses have been found to be very sensitivity to the thermal nuclear data particularly to those of ^{235}U. Recently a new experimental quantity, namely, the inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor [8] has been suggested to serve as a benchmark

quantity to check the adequacy of the ^{235}U thermal and sub thermal cross sections. By definition, the inversion point of the isothermal reactivity coefficient is the temperature where this reactor response becomes positive. According to its definition, the inversion point is believed to have the same sort of sensitivity to the thermal and sub thermal ^{235}U cross sections as the isothermal reactivity coefficient of the IPEN/MB-01 reactor does. The inversion point has been found to be adequate experimental quantity to validate calculational methodologies and related nuclear data libraries for the reactivity coefficient determination simply because its experimental determination does not require any sort of calculated correction factors or any quantity that comes either from the calculational methodologies or from another experiment. In addition to that, the inversion point is an experimental parameter that can be measured with an excellent level of accuracy and can address a specific need for benchmarking the ^{235}U thermal and sub thermal nuclear data. The purpose of this work is to perform the theoretical analysis of the inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor employing a calculational methodology based on the coupled NJOY/AMPX-II/TORT systems [9]. The nuclear data utilized in this analysis is the last release of ENDFB-VI, namely release 8 [10].

Before getting into the details of the calculational methodology, consider some physical insight of the isothermal reactivity coefficient (α_{iso}) of the IPEN/MB-01 reactor. In a recent work [7] the isothermal reactivity coefficient of the IPEN/MB-01 reactor was calculated considering a first order perturbation theory. The advantage of this approach is the sensitivity of the reactivity coefficient to the several nuclear parameters (σa_1, σa_2, etc...) and the determination of the contribution of each parameter and region to the α_{iso} calculation. Beyond that, the α_{iso} expression based on a first order perturbation theory allows one to determine the reactivity coefficient for each type of temperature, namely, the fuel temperature (Doppler effect) and the moderator temperature. The moderator temperature contribution can be further divided into two parts: the temperature of $S(\alpha,\beta)$, the thermal scattering kernel, and the moderator density (void). The final α_{iso} is obtained by summing these three contributions. Fig. 1 shows the contributions [7] of these three temperatures to the isothermal reactivity coefficient of the IPEN/MB-01 reactor for two types of nuclear data libraries. The first one (Library type A) considered ^{235}U from ENDF/B-IV and the second one (Library type B) considered ^{235}U from JEF2.2. Initially, the analyses revealed that the major difference between the reactivity coefficients calculated by libraries A and B resides in the $S(\alpha,\beta)$ temperature contribution. This contribution is positive and is bigger in the case of ^{235}U from JEF2.2. That is the main reason for the better agreement of the reactivity coefficient calculated with the ^{235}U nuclear data from JEF2.2 and it is a direct consequence of the incorporation of the new η-shape of ^{235}U [3] in the sub thermal neutron energy region in this library.

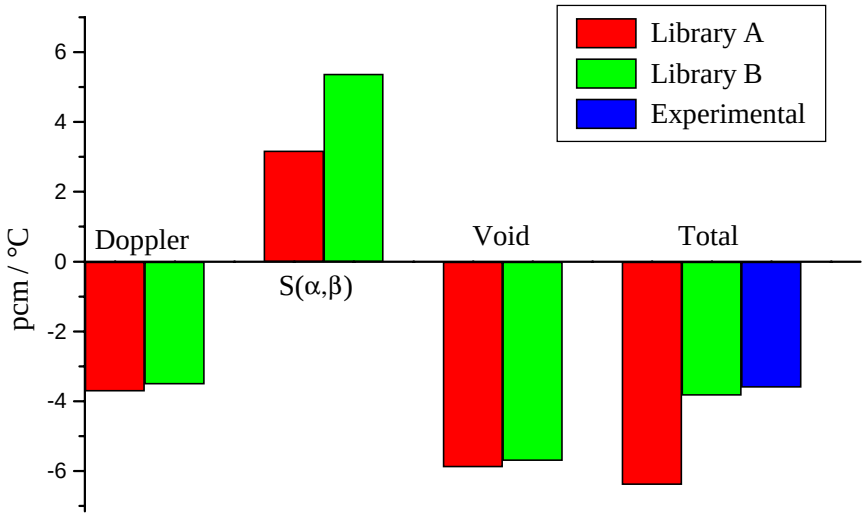


Figure 1. Temperature contributions for the isothermal reactivity coefficient of the IPEN/MB-01 reactor at 20°C.

Figure 2 shows the fuel and non-fuel region contributions to the isothermal reactivity coefficient of the IPEN/MB-01 reactor considering Library B at 20°C.

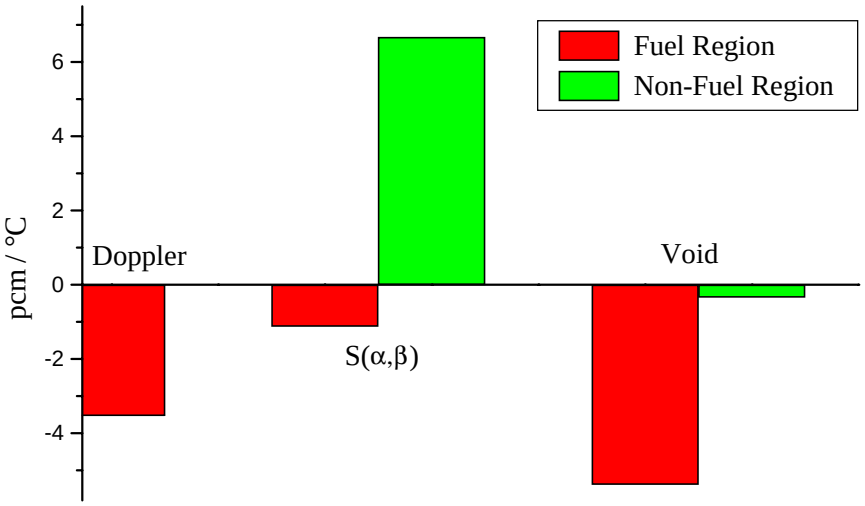


Figure 2. Temperature contributions for the isothermal reactivity coefficient of the fuel and non-fuel regions.

As shown in Fig. 2, again the major difference resides on the S(α,β) temperature contribution. The main contribution to the positive signal comes from the non-fuel region mainly from the reflector region.

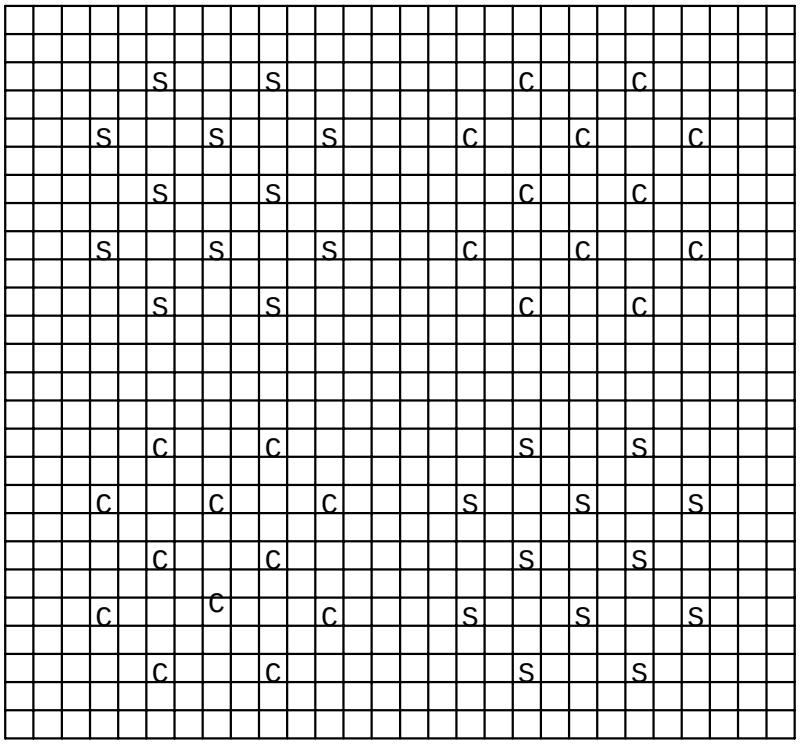
From the previous explanations it can be concluded that it is the S(α,β) temperature that gives the positive contributions for the inversion of the signal of the isothermal reactivity coefficient of the IPEN/MB-01 reactor. Particularly in this aspect the non-fuel region plays an important role.

The calculational methodology and its related nuclear data library employed for the theoretical analysis of the inversion point of the IPEN/MB-01 reactor has to cope with all the physics considerations considered in the previous analysis.

2. FACILITY DESCRIPTION

A complete description of the IPEN/MB-01 reactor is given in refs [8] and [11]. Here it will be considered the aspects of the importance to describe the core description and the experiment.

The IPEN/MB-01 reactor is a zero-power critical facility especially designed for measurement of a wide variety of reactor physics parameters to be used as benchmark experimental data for checking the calculational methodologies and related nuclear data libraries commonly used in the field of reactor physics. Fig. 3 shows its cross-section view.



C - Control Rods (Ag-In-Cd) S - Safety Rods (B_4C)

Figure 3. Cross-section view of the IPEN/MB-01 core.

The control bank at the upper right corner is named BC1 while the one at lower left corner is named BC2. The control/safety bank position is given in percentage withdrawn. The reference level or zero for the withdrawn position occurs when the bottom of the active absorber length (including the bottom plugs) is aligned with the bottom of the fuel region. The uppermost position (100% withdrawn) is the top of the fuel region. During the reactor operation, both of the safety banks are kept far away from the 100% withdrawn position, and the control banks can both be withdrawn from the bottom of the fuel region, but the final criticality control is made with just one of them.

3. EXPERIMENTAL PROCEDURE

A complete description of the experiment of the inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor can be found in Ref. [8]. Here it will be considered just a few details in order to give some insight into the experiment as well as to illustrate the theoretical modeling of the reactor system. The moderator bank was initially filled with water at 8.5°C, and the reactor system was allowed to reach thermal equilibrium. The control bank BC2 was always kept at the 58.5% withdrawn position, and the fine criticality control was achieved by the automatic control system continuously positioning the control bank BC1 around the fine critical position. Fig. 4 shows schematically the control bank configuration for the experiment.

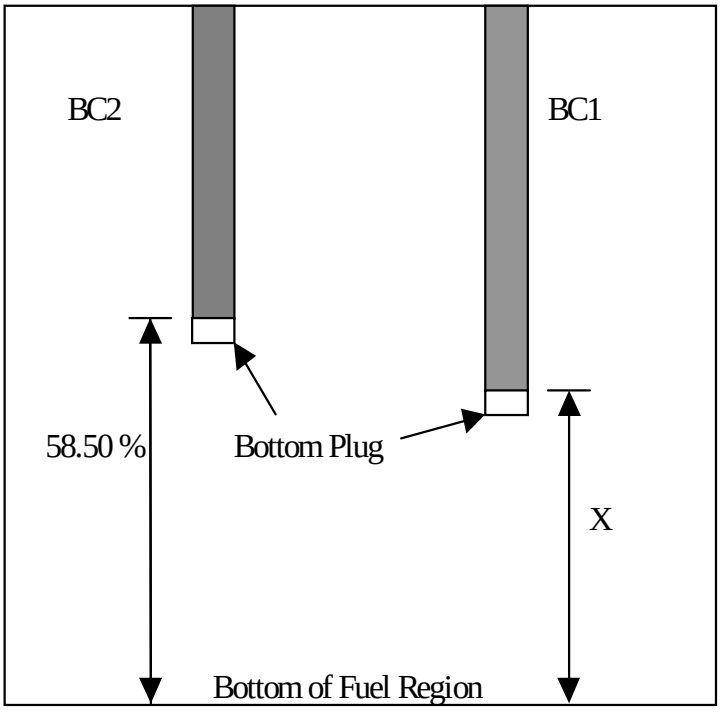


Figure 4. Schematic axial representation of the control bank position.

The moderator water was slowly heated up to ~ 25°C by a heating/cooling system in a stepwise manner in order to achieve a maximum temperature variation of ~ 0.5°C between successive data acquisitions.

Extreme care was taken to guarantee the temperature homogenization in the reactor. The systematic and statistical uncertainties were taken into consideration in the analysis of the experimental data by an appropriate procedure.

4. CALCULATIONAL METHODOLOGY

The calculational methodology applied for the analyses of the inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor is shown in Fig. 5. Basically, starting from ENDF/B-VI.8 nuclear data library, the well known NJOY system (version 97.115) [12] was employed to access and to process this nuclear data file in a fine group structure. The thermal scattering law for hydrogen bound in water was obtained with LEAPR module of NJOY.

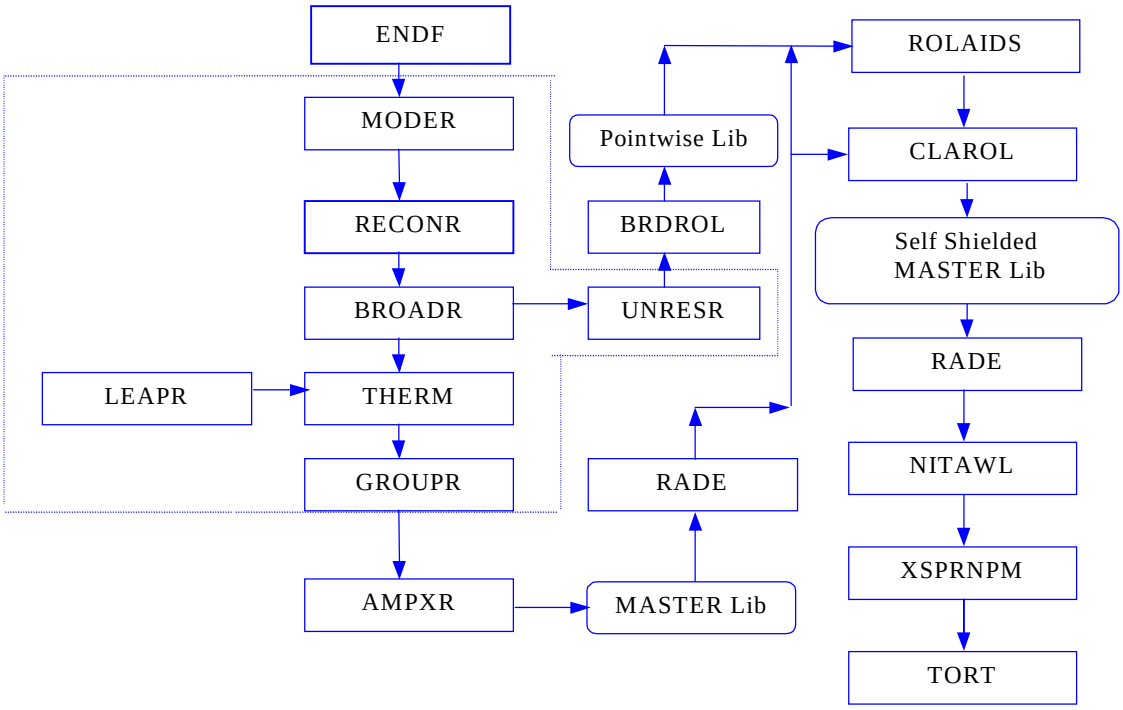


Figure 5. Schematic diagram for the deterministic calculational methodology.

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 [13] package. The pointwise and fine multigroup cross sections produced in the previous step are transferred to AMPX-II by two in house interface modules BRDROL and AMPXR. The self-shielding treatment of the actinide resolved resonances in the neutron energy region from 0.600 eV to 5.50 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, guide tube, and bottom plugs were obtained using a super-cell model. At this point, the cross section library is problem dependent. XSDRNPM was run in a S_{64} quadrature set. The procedure considered a fine multigroup of 620 groups (SAND-II structure) as recommended in Ref. [9]. This set of fine multigroup library was collapsed to 16 groups (5 upscaterring in the thermal range) as again recommend in Ref. [9]. The order of scattering (Legendre order expansion) was P_3 throughout the analysis. Finally, the broad group library is conveniently formatted to the TORT (3D Discrete Ordinates Code) [14] format using the GIP [15]program. Subsequently, using the cross sections libraries generated before, TORT performed K_{eff} calculations considering a fully three-dimensional geometric modeling of the IPEN/MB-01 reactor core.

The fully three-dimensional geometric setup for the TORT calculations was considered with the X-Y-Z geometry, P_3 approximation, angular quadrature S_{16}, and 16 groups of energy. 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 210,600 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 1.00E-05 for the flux and the fission source and 1.00E-06 for the eigenvalue.

This whole pattern of calculations (cross section generation and the subsequent TORT K_{eff} calculations) was considered for the entire temperature interval spanning from 20ºC to 4°C. The calculations were considered for every interval of 2°C; more precisely the cross section generation and the TORT K_{eff} analysis were performed at 20°C, 18 °C, 16°C and so forth up to 4°C. Since the final result is the reactivity variation as a function of the temperature, the procedure here was to keep the control rod positions at 20°C for all other temperatures and to calculate the reactivity variation as the temperature changes relatively to the case of 20°C.

However a lot of details in the calculational methodology have to be adapted to cope with the task of the analysis of the inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor. First of all, since the reactivity, temperature, and cross section variations are small all the computer codes were transformed to DOUBLE PRECISION. The RECONR, BROADR and THERMR modules of NJOY were run with 0.2%, 0.1% and 0.1%, interpolation tolerance criterion respectively for all nuclides. The convergence criterion for all XSDRNPM runs were set to 1.0E-06. TORT was run considering a convergence criterion of 1.0E-05 for the

neutron flux and fission source and 1.0E-06 for K_{eff}. Furthermore, during the analysis it was found TORT was very sensitive to the number of digits used for the final weighted cross section written by XSDRNPM (ANISN Format). The default value is 5 digits. Several calculations were performed in order to analyze this effect. Figs 6 and 7 summarizes the main conclusions when this number of digits was increased to 7 in the XSDRNPM source program. Fig. 6 shows the TORT K_{eff} as a function of the XSDRNPM quadrature order considering 5 and 7 digits for the ANISN cross sections considering the system temperature equal to 14°C. It can be seen in this figure that TORT K_{eff} stabilizes for the case of 7 digits. Fig. 7 shows the TORT reactivity relative to the 20°C case as a function of temperature considering 5 and 7 digits for the ANISN cross sections. Here, the impact of the number of digits of the ANISN library is more severe. It can be noted clearly the best performance of the case considering 7 digits. The curve is much smother. One last consideration was the number of emerging energies for the secondary neutrons emitted in a scattering considered by THERMR. This number is set at 59 emerging energies independent of the nuclide and of the nuclear process. Since the thermal scattering for Hydrogen bound in water is crucial for the problem under consideration in this work, this number of emerging energies was increased to 948. The energies considered were the ones obtained from the linearization of the Hydrogen cross sections at the thermal energies.

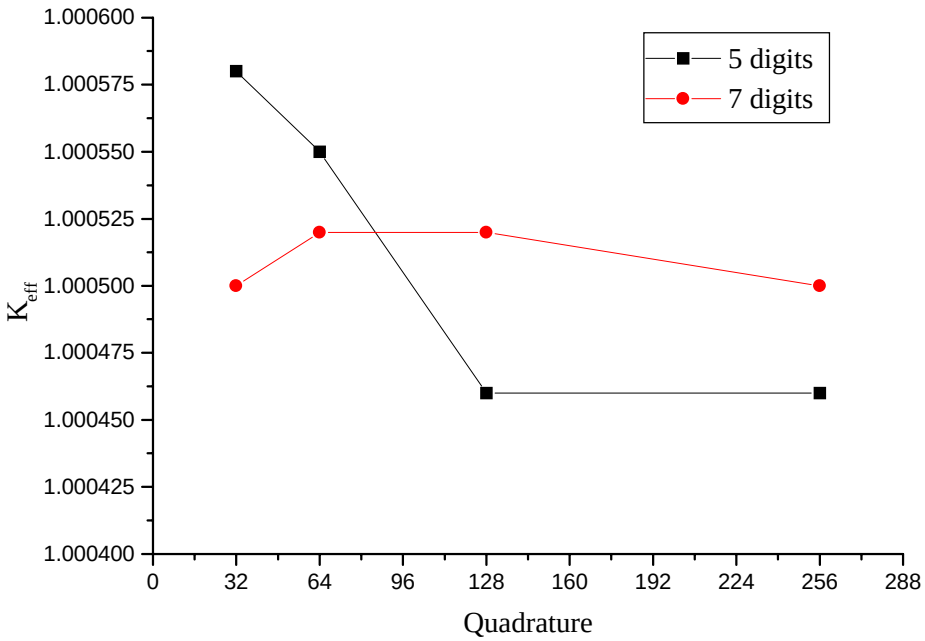


Figure 6. TORT K_{eff} as a function of the XSDRNPM quadrature order considering 5 and 7 digits.

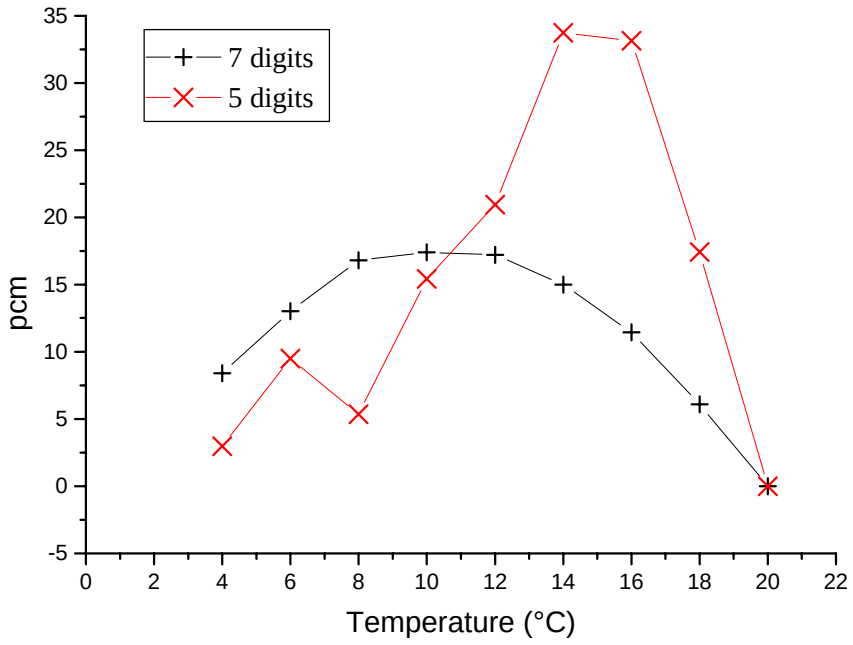


Figure 7. TORT reactivity considering 5 and 7 digits in the ANISN library.

5. RESULTS AND DISCUSSIONS

The final results for the reactivity as a function of temperature is shown in Fig. 8. This figure shows the calculated reactivity variation as well as the critical BC1 control bank position both as a function of the temperature.

The inversion point in both curves is obtained at the temperature where the curve shows a maximum for the reactivity (theoretical model) and a minimum for the critical BC1 control bank position (experimental value). The theoretical value is 10.53°C while the experimental value for the inversion point is 14.99±0.15 °C. There is a difference of 4.58°C. This difference is positive which is consistent with the underprediction of the calculated isothermal reactivity coefficient. The calculated reactivity coefficient is smaller than the experimental [7]. At first glance it appears to be a considerable discrepancy. However from the experimental curve of the isothermal reactivity coefficient of the IPEN/MB-01 reactor [7] one may note that for every 1°C variation in the temperature scale there is a variation of nearly 0.2 ± 0.01 pcm/°C in the reactivity coefficient. Therefore, for a variation of 4.46°C there is a variation of -0.89 ± 0.05 pcm/°C in the reactivity coefficient which shows that this deviation is inside of the desired accuracy [16] (-1.0 pcm/°C) for the calculation of the reactivity coefficient. In this aspect, the whole methodology and the related nuclear data library (ENDF/B-VI.8) attain the desired accuracy for the isothermal reactivity calculation.

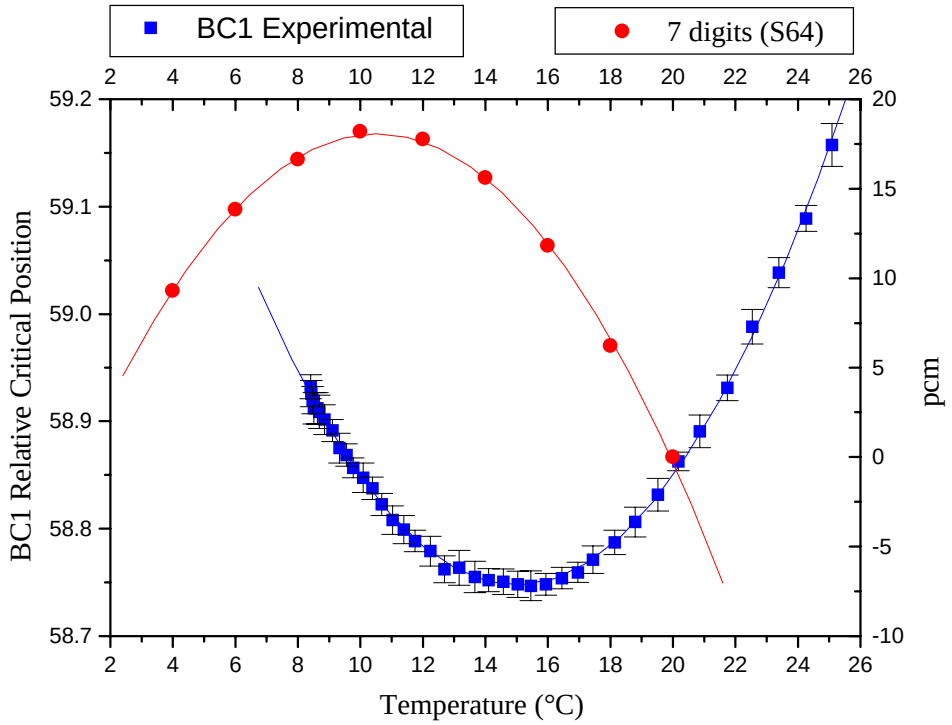


Figure 8. Calculated reactivity variation and experimental critical BC1 control bank position as a function of the temperature.

6. CONCLUSIONS

The theoretical analyses of the inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor have been successfully accomplished. The analyses reveal that for this peculiar problem TORT is very sensitive to the number of digits utilized in the ANISN library written by XSDRNPM. The theoretical analysis performed in this work can be considered a real challenge in the reactor physics field due to the peculiarities of inversion point of the isothermal reactivity coefficient of the IPEN/MB-01 reactor. The experiment itself as extensively described in Ref. 8 was also considered a real challenge and its successful completion can be credited mostly to the very accurate control system characteristics of the IPEN/MB-01 reactor. The reader must realize from Fig.8 the very small range of the BC1 critical positions. The analysis also reveals that the new η-shape of ^{235}U improves the theory/experiment agreement and even more gave an indication that the desired accuracy for the isothermal reactivity calculation for thermal reactors has been achieved.

REFERENCES

1. L. C. Leal, G. de Saussare, and R. B. Perez, “An **R** Matrix Analysis of the ^{235}U Neutron-Induced Cross Sections up to 500 eV,” *Nucl. Sci. Eng.*, **109**, pp.1-17 (1991).

2. L. C. Leal, H. Derrien, N. M. Larson, and R. Q. Wright, "R-Matrix Analysis of ^{235}U Neutron Transmission and Cross Section in the Energy Range 0 to 2.25 keV," ORNL/TM-13156, Oak Ridge National Laboratory (Nov. 1997).
3. H. Weigmann et al., "Measurements of η of ^{235}U for Sub-Thermal Neutron Energies," *Proc. Conf. Physics of Reactors: Operation, Design, and Computation, Physor-90*, Marseille, France, 23-26 April 1990, Vol. P I , pp. 33-41 (1990).
4. A. dos Santos, R. Fuga, R. Jerez, A. Y. Abe, and E. A. Filho, "A Proposal for Benchmarking ^{235}U Nuclear Data," *Nucl. Sci. Eng.*, **137**, pp.52-69 (2001).
5. A. dos Santos, "Some ENDF/B-VI Benchmark Results," *Trans. Am. Nucl. Soc.*, **76**, pp. 332-333 (1997).
6. C. Mounier, "Contribution a Létude du Coefficient de Temperature des Reactures a Eau Legere," CEA-N- 2761, Commissariat à l`Energy Atomique (1994).
7. A. Santos, H. Yoriyaz, R. Fuga, and R. Jerez, "Reactivity Coefficient of IPEN/MB-01 Reactor," *Proc. Int. Conf. Physics of Reactors, Physor-96*, Mito, Ibaraki, Japan, 16-20 September 1996, Japan Atomic Energy Research Institute (1996).
8. A. Santos, H. Pasqualeto, L. C. C. B. Fanaro, R. Fuga, and R. Jerez, "The Inversion Point of the Isothermal Reactivity Coefficient of the IPEN/MB-01 Reactor—1: Experimental Procedure," *Nucl. Sci. Eng.*, **133**, pp. 314-326 (1999).
9. A. dos Santos, A. Y. Abe, A. G. Mendonça, L. C. C. B. Fanaro, and G. S. Andrade e Silva, " Criticality Analysis Based on the Coupled NJOY/AMPX-II/TORT Systems," *Proc. Int. Conf. Physics of Nuclear Science and Technology*, Pittsburgh, Pennsylvania, 7-12 May 2000, American Nuclear Society (2000).
10. " ENDF/B-VI Summary Documentation," BNL-NCS-17541 (ENDF-201), 4th ed. (ENDF/B-VI), P. F. Rose, Ed. , National Nuclear Data Center, Brookhaven National Laboratory (Release-8 2002).
11. A. Santos, H. Pasqualeto, R. Fuga, R. Jerez, and A. Y. Abe, "A Contribution for Benchmarking ENDF/B-VI Isothermal Reactivity Coefficient Determination," *Proc. Int. Conf. Physics of Nuclear Science and Technology*, Long Island, New York, 5-9 October, 1998, American Nuclear Society (1998).
12. R. E. MacFarlane, D. W. Muir, R. M. Bouicort, "NJOY – Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Section from ENDF Data," LA-12740-M, Los Alamos National Laboratory (1994).
13. N. M. Greene, et al, "AMPX-II: A Modular Code System for Generation Coupled Multigroup Neutron-Gamma Libraries from ENDF/B," ORNL-TM-3706, (1976).
14. W. A. Rhoades, D. B. Simpson, "The TORT Three-Dimensional Discrete Ordinates Neutron/Photon Transport Code," ORNL/TM-13221, (1991).
15. W. A. Rhoades, "The GIP Program for Preparation of Group-Organized Cross Section Libraries," ORNL, (1975).
16. J. Bouchard, C. Golinelli, and H. Tellier, "Besoins en Donneés Nucléaires pour les Réacteurs a Neutron Thermique," *Proc. Int. Conf. Nuclear Data for Science and Technology*, Dordrecht (Netherlands), 6-10 September 1982, Vol. 1072, pp. 21-28, (1983)