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Implementation And Application of RCP System at BNL*

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Abstract

We will discuss the implementation of the RCP01 Monte Carlo system at the Brookhaven National Laboratory Central Scientific Computing Facility. Initial benchmarking experience and an LWR core physics application will be described.

1. Introduction

The RCP01[1] program is a generalized three dimensional continuous energy Monte Carlo program suitable for thermal reactor benchmark calculations. A library preparation program (RCPL1)[2] exists for creating Doppler broadened cross section profiles for use in RCP01 after they have been processed from ENDF/B source tapes. These programs were written at the Bettis Atomic Power Laboratory (BAPL) and first distributed in the late 1970's through the National Energy Software Center at Argonne.

2. Implementation

2.1 XAP Cross Section Data From ENDF/B

The XAP data base concept frees the casual RCP01 user from the complexities of the ENDF/B storage and processing programs. Data is arranged into two distinct structures (fast and thermal) before any Doppler broadening of resonances occur. Thus, any given isotope need only be processed once from ENDF/B to each XAP database. Modified versions of the standard programs ETOG,[3] ETOT,[4] and FLANGE[5] are used for this transformation. Since XAP uses AFM (See 2.3) which in turn uses standard software, these databases can be stored online when constructing specific libraries. Currently, at BNL we have 20 nuclides and 5 kernels on our XAP databases. It has been our policy only to add nuclides to the databases on an "as needed" basis. The information in XAP when needed by RCPL1 is retrieved by random access read routines based on isotope, energy group, reaction type and subtype (if any). A backup to the random database consists of UPDATE files necessary to regenerate the information. Thus, once all the nuclides needed for a study are contained in XAP only a single RCPL1 library generation job will provide the needed broadened pointwise library in AFM format.

The overall structure of what we will call the RCP system is shown in Figure-1. The modified versions of the standard ENDF/B processing codes given in Level I of Figure-1 provide data to the XAP libraries of Level II. The XAP thermal and epithermal libraries then provide multigroup cross section data and resonance parameters which may be used by other calculational tools as well as by RCP01. The XAP libraries contain epithermal multigroup averaged and thermal mid-group cross sections, as well as parameters needed to calculate resonance cross section profiles for resonance nuclides. RCPL1 then prepares

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the cross section job library for RCP01 by using data in the XAP libraries. It accesses the resolved resonance parameters and forms profiles by whatever formalism is dictated and then Doppler broadens them. It creates an unresolved resonance distribution based on a Porter-Thomas distribution. Appropriate thermal kernels and smooth data are also digested.

2.2 Cross Section Data For RCP01

The data produced by RCPL1 consists of both multigroup and point data. Smooth integral cross sections are given as multigroup sets within a relatively arbitrary energy structure (in practice, the epithermal data is given for 54 multigroups and the thermal data is given for 25 multigroups). Doppler broadened cross sections for resonance nuclides are obtained from unresolved and either (symmetric or asymmetric as appropriate) Breit-Wigner single-level, or Adler-Adler or Reich-Moore, multi-level parameters. These cross sections are tabulated on a user prescribed fine energy mesh within the RCP group structure. The fine energy mesh is nuclide independent. The energies selected for the pointwise resonance cross sections are uniformly spaced between the energy breakpoints of the group. Unresolved resonance regions are treated by generating a random sample cross section set on a fine energy mesh, in a preprocessor stage, which is then handled in a manner that is similar to the resolved resonance data in RCP01 but preserves the characteristics of the Porter-Thomas distribution that was used to sample the unresolved structure. Pointwise data includes microscopic capture, elastic scattering and fission cross sections. Each XAP resonance nuclide may be a multi-isotope mixture of as many as 25 components. This considerably simplifies the representation of structural materials such as Zircaloy, stainless steel, etc.

Differential nuclear data is usually in a multigroup form with the multigroups related to the group structure used in the RCP01 calculation. Inelastic scattering (permitted only in the highest energy groups) is assumed to be isotropic in the center-of-mass system (CMS) and is treated via multigroup scattering matrices. Elastic scattering is described by the first four Legendre components of the differential cross section in the CMS. Elastic scattering may be anisotropic in the inelastic scattering groups, but is assumed to be isotropic in the CMS in all other epithermal groups. Scattering from bound Hydrogen is assumed to be from a free proton at rest in the epithermal groups, except for the Special Epithermal Treatment which may extend over some of the lowest epithermal RCP groups. In that case the bound Hydrogen target is treated kinematically as a free proton target with a Maxwellian distribution of velocities corresponding to an effective "source" temperature.

In the thermal group, P-3 25 group scattering kernels are used for the treatment of neutronic interactions with up to two non-resonance nuclides. Each kernel consists of four transfer matrices describing the scattering of neutrons among the thermal subgroups. However, only one kernel is allowed in a given material.

2.3 Software Implementation

The specialized system required for this environment[6] is not the standard CDC-7600 suplied software. The BAPL environment can for the most part be simulated on standard CDC operating systems by using the MODEL[7] environment. The major BNL programming effort involved (a) writing an advanced file manager (AFM) simulator to interface with standard CDC permanent filing and (b) writing the data base retrieval routines (XAP) to interface with AFM in a truly random read-write capability for cross section and parameter isotopic information.

RCP01 needs AFM both to read the cross section library and to write and read files for restart and editing. No other major changes in the program environment were necessary for execution on a CDC 7600 except the interface to a plotting package. Minor inadequacies in the SCOPE 2.1.5 overlay loader necessitated some trivial changes in the overlay structure of RCP01 enabling the entire system to enter a preproduction Q/A phase at BNL.

3. Applications

The RCP01 system described above has been used in various applications in BNL's Light Water Reactor Safety activities. The system performance was first evaluated by simulating some experimental and calculational benchmarks. Results were then compared either to the experiments or to the results obtained from other Monte Carlo analyses. These calculations verified that the cross section generation procedures and the Monte Carlo simulation had been properly implemented, and that consistent results were obtained. After the successful benchmarking, a calculation of incore detector activation and local fission rate distribution was performed for a typical PWR assembly. RCP01 results were then compared to results obtained from deterministic design codes.

3.1 Benchmarking

Calculations of critical experimental benchmarks are often used to qualify a specific computational approach for the solution of a class of problems whose characteristics are similar to those of the experimental configuration. Comparison of the calculated and experimental results helps to quantify the deviation of the calculated result from experimentally measured "truth."

Benchmarking calculations were performed for the Cross Section Evaluation Working Group (CSEWG) TRX-1 unit cell benchmark and two Battele Pacific Northwest Lab (PNL) fuel storage rack critical experiments.[8] Cross section job libraries were generated at room temperature for the required isotopes using ENDF/B-V based data and the procedures described previously.

3.1.1 TRX-1 Unit Cell

The TRX-1 critical benchmark experiment was performed years ago at the Bettis Atomic Power Laboratory. It consisted of a uniform hexagonal lattice of slightly enriched (1.3 wt.% U-235) Uranium metal rods in a H_2O moderator. The rods were clad in Aluminum and had a 0.5753 cm O.D. on a 1.806 cm triangular pitch. The experiment was done at room temperature. This simply buckled configuration has long been used as a standard for testing spectrum codes and is one of the most heavily used benchmarks by the CSWEG.

In the RCP01 calculations we modelled one-third of the unit cell, with the fuel, gap and clad explicitly represented, and with ENDF/B-V based nuclear data. Approximately 38,000 neutron histories were processed. The results obtained for the infinite multiplication factor and for various measured reaction rate ratios are shown in Table-1. The breakpoint between "fast" and "thermal" energies was assumed to be 0.625 eV. The quoted 1σ uncertainties assume no correlation between the estimates for the reaction rates. Table-1 also shows the experimentally measured quantities, as well as the results obtained from two other state-of-the-art Monte Carlo codes - SAM-CE[9] and MCNP[10] also using ENDF/B-V. The principal differences between these codes is in the modelling of nuclear data - both SAM-CE and MCNP use essentially pointwise data and explicit treatments of thermal scattering (S (α,β) while the RCP01 nuclear data are based on mixed group and point formalisms as described above.

The results show excellent agreement between the results from the three Monte Carlo codes, and good agreement with experiment. It should be noted that the indicated levels of agreement with experiment generally represent considerable improvement over the comparable results obtained with ENDF/B-IV based nuclear data.[11]

3.1.2 Fuel Storage Pool Criticals

The storage pool experiments that were simulated involved the determination of the critical separation between three clusters of UO_2 rods arranged in a linear array, both with and without 1.1 wt % borated stainless steel absorber plates located between the clusters.[8] The clusters consisted of 15 x 8 arrays of 4.31 wt % enriched UO_2 rods (clad in Aluminum) at a lattice pitch of 2.54 cm. With this fuel and lattice spacing, a critical configuration can be achieved with a single 8 x 16.37 $\pm$ 0.03 cluster. The configurations that were examined therefore represent a loosely coupled system, and are a strigent test for any calculational approach.

The analyses were performed with two continuous energy Monte Carlo programs, SAM-F (the Monte Carlo component of the SAM-CE system) and RCP01, using nuclear data based on ENDF/B-V. The cross setion library for SAM-F was obtained from the National Nuclear Data Center. The experimental configurations were modelled in detal with both programs (i.e. fuel-gap-clad, absorber plates, and the surrounding water filled tank). The structural materials within the tank, and the tank itself were not explicitly modelled, but this omission is expected to have a negligible effect on the calculated results. Approximately 20,000 neutron histories were processed for each simulation.

The results obtained for the critical configuration in the absence of the poison plates, and with the borated stainless steel plates present are presented in Tables 2 and 3, respectively. The SAM results utilize the Maximum Likelihood Estimator.[11] The number of neutron histories processed per minute on a CDC-7600 are presented for the SAM and RCP results as a measure of the efficiency of the Monte Carlo simulation. Results obtained with KENO-IV (from Ref. 12) using three cross section libraries (27-group ENDF/B-IV; 123-group GAM-THERMOS; 16-group Hansen-Roach) are also presented. The KENO calculations involved the processing of approximately 30,000 neutron histories, but no information is available on the computing times.

3.1.3 Conclusions From Benchmark Calculations

The results shown in Tables 1-3 support the following conclusions about the performance of RCP01, with ENDF/B-V data, for systems similar to those encountered in analyses of light water reactors (LWRs):

1. RCP01 performs well relative to experiment, and relative to other Monte Carlo codes that are available for LWR related analyses.

2. RCOP1 is approximately twice as fast, for comparable accuracy, as SAM-CE (cf.Table-2).

3.2 Calculation of Fission Rates For Typical PWR Assembly

Following the successful benchmarking of RCP01 for LWR related systems, a comparison was made between results obtained from different calculational approaches for the in-core detector activation rate-to-local and global fission rates in a typical PWR assembly. The objective of the study was to compare results from standard design codes to results obtained from a detailed calculation performed with a continuous energy Monte Carlo program (RCP01) with ENDF/B-V based nuclear data.

Calculations were performed for a typical PWR type assembly at BOL using three distinct calculational methods:

1. Use of a transport theory based multigroup spectrum code to obtain spatially homogenized, energy condensed cross sections for distinct regions in the lattice, followed by a few-group diffusion theory calculation for a partially homogenized assembly. This approach is embodied in the use of the EPRI-CELL[13] and PDQ-7II[14] programs, and is typical of the methods generally used to perform this type of calclation.

2. Similar to (1), except that the assembly calculation utilizes transport theory. This approach is embodied in the CASMO[15] program, and represents a more sophisticated treatment of the problem.

3. A Monte Carlo calculation for the assembly which retains all the spatial and energy detail. This approach is available in the RCP01 program. Since it involves minimal approximations, it serves as the reference calculation.

Fission rates for the assembly and for the fission chamber detector are summarized in Table 4. Results are normalized to a total production rate of unity for the assembly, and are presented separately for the fissioning isotopes, and for the fast and thermal energy ranges, as well as the sum over all energies.

Fission rate distribution and eigenvalue results are presented in Figure-2. The total 1σ uncertainties from RCP01 associated with each of the local fuel rod fission rates are shown. The quoted uncertainties consist of two components: 1) the uncertainity in the Monte Carlo estimate of the fuel rod fission rate, and 2) an estimate of the uncertainty associated with the eigenfunction. Note that the uncertainties for locations not on the symmetry axes are lower than the values on the vertical and 45° axes. This is because fissions in two symmetrically located rods are involved in the estimates for these loctions. Figure 2 also shows the percent differences between the RCP01 mean estimates for the normalized local fission rates, and the results from the deterministic methods. Although there are some locations where these differences are greater than the 1σ uncertainty in the Monte Carlo results, when a 2σ range is considered (corresponding to approximately a 95% confidence interval) the results from the three calculations "agree" in most locations.

RCP01 predicts the highest eigenvalue for the configuration, consistent with the use of ENDF/B-V data. The PDQ-7II eigenvalue is lower (as expected since pre-ENDF/B-V data are involved) but is within the 1 uncertainty on the Monte Carlo results. The CASMO eigenvalue is the lowest of the three. This result is consistent with the level of agreement that was observed in an earlier study between PDQ-7II and the CPM program (which is very similar, in terms of results, to CASMO).[16]

The Monte Carlo results involved the processing of 99,710 neutron histories, resulting in 1 uncertainities of $\sim$1.5-3.0% (cf. Figure-2) for the individual fuel rod fission rates and $\sim$7-8% for the detector fission rate.

There is generally good agreement between the results from the three methods in terms of the integrated fission rate for the assembly as a function of both isotope and energy (cf. Table 4). There is also reasonable agreement between all three methods in terms of the fission rate distribution for the assembly (cf.Fig. 2).

Agreement between E-CELL/PDQ-7II and CASMO for the detector fission rate is also good, but both methods predict a much higher fission rate than does RCP01 (~15-19% higher). There are a number of possible reasons for this discrepancy, including differences in modelling the assembly geometry, and differences in the treatment of nuclear data (especially at the assembly level). In particular, the modelling differences give rise to a much larger absorption rate in the instrument thimble surrounding the detector in the RCP01 model (by 14%); hence fewer thermal neutrons are available to cause fissions in the U-235 in the detector location.

The results obtained during the course of this study provide increased confidence that fission rate distributions for PWR assemblies are being well calculated by standard design techniques. The discrepancies observed between results from Monte Carlo calculations, and those obtained from standard design codes for the detector fission rate, suggest that further studies in this area are desirable.

4. Conclusions

Thus, in its first years since its release from the cloistered environment of the BAPL operating system, we have successfully implemented RCP01 on standard CDC software, benchmarked it, and begun to use it in mission oriented LWR safety work. In the future as the needs arise, the databases will be enlarged to encompass more isotopes. Geometry decks of various common configurations will be generated and available. At that time the RCP01 package will be available to quickly answer safety problems with a high quality solution.

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FIGURE 1

RCP ENDF/B DATA FLOW

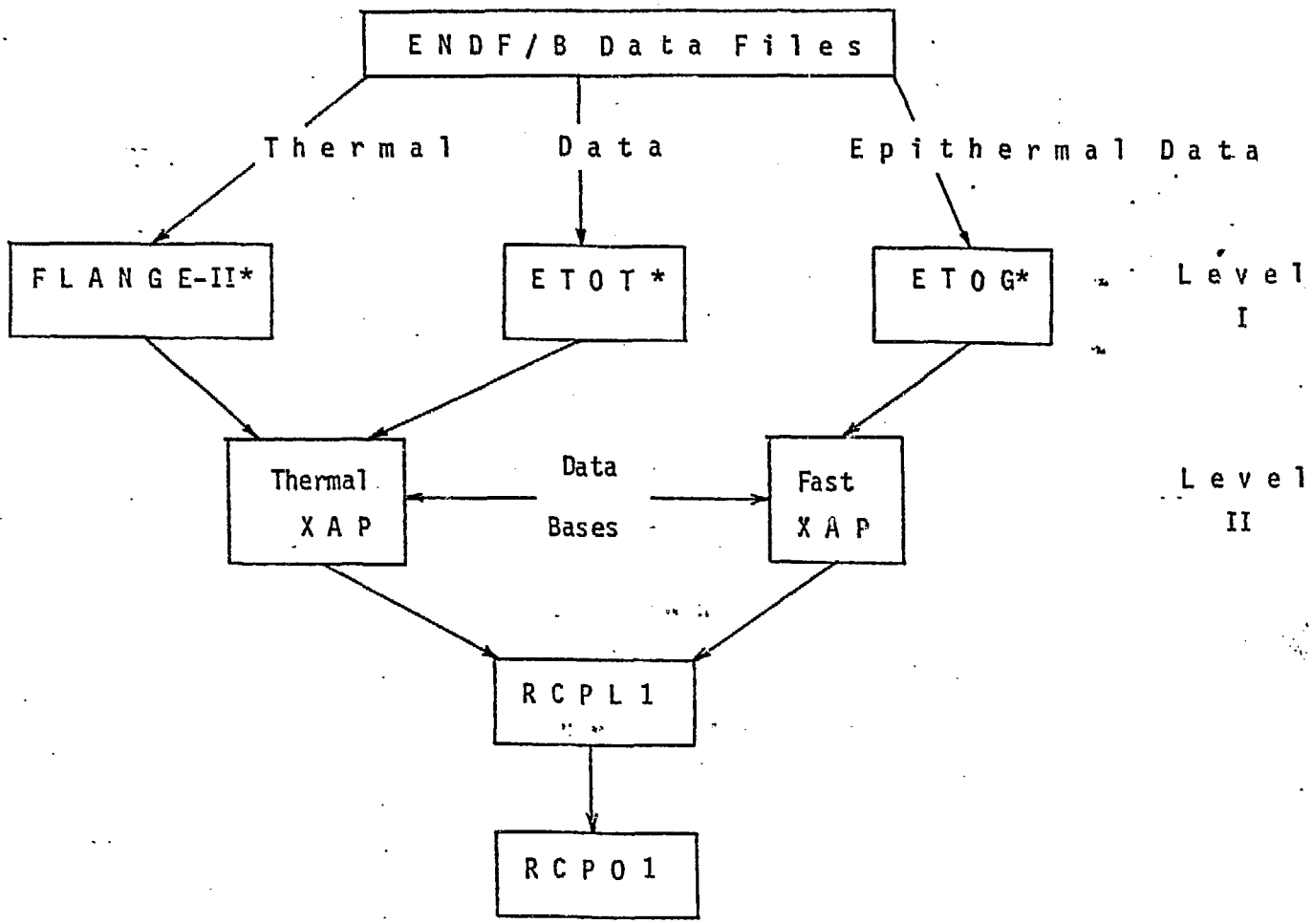

FIGURE 2

One Standard Deviation Uncertainties On RCP01 Local Fission Rates; and Percent Differences Between RCP01 Mean Estimates For Normalized Fission Rates and CASMO and PDQ-7II Results

2.7 0.5 1.0	2.7 -0.1 0.4	% % %	RCP01 Difference CASMO vs. RCP Mean Estimate Difference PDQ vs. RCP Mean Estimate					
2.7 2.6 3.3	1.6 -0.6 0.0	2.6 -1.2 -0.4						
	1.9 1.6 1.1	1.9 -2.1 -2.2						
2.6 0.5 0.5	1.9 -0.9 -0.1	1.7 2.6 3.6	2.2 -1.7 -1.4	2.7 4.6 6.6				
2.6 0.7 1.6	1.9 -1.4 -0.6	1.9 -2.4 -1.5	1.9 -1.3 -1.0	2.2 -0.6 0.2				
	2.2 -0.5 -1.0	1.9 -0.8 -1.1		1.6 0.8 1.2	1.6 -0.7 -1.0	2.7 -1.2 -1.0		
2.6 0.0 0.3	1.7 3.2 3.6	2.0 -0.1 0.2	1.9 -2.9 3.4	2.0 -0.5 -0.2	2.0 -2.8 -3.2	1.7 1.9 1.1	2.8 0.1 -1.0	
2.7 0.8 0.8	2.0 0.3 -0.1	1.7 1.0 0.4	1.7 1.8 1.2	2.3 -4.1 -4.8	1.7 -0.4 -1.4	2.1 2.2 1.1	1.8 2.8 1.4	2.8 3.6 2.0

k RCP01) = 1.131 + 0.002
k (CASMO) = 1.122
k (PDQ-7) = 1.129

TABLE-1

RESULTS FOR TRX-1 CELL
BENCHMARK
ENDF/B-V NUCLEAR DATA

PARAMETER	EXPERIMENT	RCP01
k_∞	--	1.1840 ± 0.0030
ρ_{28}	1.311 ± 0.02	1.312 ± 0.010
δ_{25}	0.0981 ± 0.001	0.0969 ± 0.0012
δ_{28}	0.0914 ± 0.002	0.0912 ± 0.0008
C*	0.792 ± 0.008	0.786 ± 0.002

	SAM-CE*	MCNP*
k_∞	1.1847 ± 0.0012	1.1800 ± 0.0008
ρ_{28}	1.300 ± 0.007	1.318 ± 0.005
δ_{25}	0.0947 ± 0.0004	0.0966 ± 0.0003
δ_{28}	0.0913 ± 0.0004	0.0912 ± 0.0004
C*	0.782 ± 0.002	0.788 ± 0.002

* COMMUNICATED BY E. SCHMIDT - BNL-NNDC

TABLE 2

MONTE CARLO RESULTS FOR
SIMULATION OF UNPOISONED
CRITICAL

METHOD	$K_{EFF} \pm 1^{\sigma}$	# NEUTRON HISTORIES MIN.
RCP01	0.9996 ± 0.007	1413
SAM-F	1.0052 ± 0.007	694
KENO-IV		
LIBRARY 1*	0.989 ± 0.005	
LIBRARY 2*	0.984 ± 0.004	NOT
LIBRARY 3*	0.997 ± 0.004	AVAILABLE

*KENO-IV LIBRARIES ARE ALL MULTIGROUP (RESULTS ARE FROM REFERENCE 5)

LIBRARY 1 - 27-GROUP ENDF/B-IV

LIBRARY 2 - 123-GROUP GAM-THERMOS (ENDF/B-II)

LIBRARY 3 - 16-GROUP HANSEN-ROACH

TABLE 3

MONTE CARLO RESULTS FOR
SIMULATION OF POISONED
CRITICAL

METHOD	$K_{EFF} \pm 1\sigma$	#NEUTRON HISTORIES / MIN.
RCP01 +	1.003 ± 0.009	1404
SAM-F	0.996 ± 0.004	734
KENO-IV		
LIBRARY 1*	0.982 ± 0.004	
LIBRARY 2*	0.987 ± 0.004	NOT
LIBRARY 3*	1.001 ± 0.004	AVAILABLE

* KENO-IV LIBRARIES ARE ALL MULTIGROUP (RESULTS ARE FROM REFERENCE 5)

LIBRARY 1 - 27-GROUP ENDF/B-IV

LIBRARY 2 - 123-GROUP GAM-THERMOS (ENDF/B-II)

LIBRARY 3 - 16-GROUP HANSEN-ROACH

+ RESULTS FOLLOWING PROCESSING OF 9500 NEUTRON HISTORIES

TABLE 4

Summary of Detector And Assembly Fission Rates

	RCP01	CASMO	PDQ-7II
Assembly Fission Rates			
U-235 Fission Rate			
Fast*	5.76(-2)+	5.93(-2)	5.84(-2)
Thermal*	3.21(-1)	3.22(-1)	3.22(-1)
Total*	3.79(-1)	3.81(-1)	3.81(-1)
	(± 0.33% 1σ)		
U-238 Fission Rate			
Fast	2.74(-2)	2.70(-2)	2.70(-2)
Thermal	1.18(-7)	0.0	0.0
Total	2.74(-2)	2.70(-2)	2.70(-2)
	(± 0.42% 1σ)		
U-235 + U-238 Fission Rates			
Fast	8.50(-2)	8.64(-2)	8.54(-2)
Thermal	3.21(-1)	3.22(-1)	3.22(-1)
Total	4.06(-1)	4.08(-1)	4.08(-1)
	(± 0.31% 1σ)		
Dectector Fission Rates			
U-235 Fission Rate			
Fast	2.21(-11)	2.22(-11)	2.27(-11)
Thermal	1.03(-10)	1.27(-10)	1.22(-10)
Total	1.25(-10)	1.49(-10)	1.45(-10)
	(± 7% 1σ)		

*Fast refers to energy range 10 MeV-0.625 eV
Thermal refers to energy range 0.625 eV-0.0 eV
Total refers to energy range 10 MeV-0.0 eV

+ Read as 5.76×10^{-2}