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THE FRENCH "CEA 86" MULTIGROUP CROSS-SECTION LIBRARY AND ITS INTEGRAL QUALIFICATION

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ABSTRACT

This paper describe the up-dated 99 groups library of the APOLLO French neutron computer code, the denominated "CEA 86" library. The multigroup cross-section sets are based on the more recent nuclear data evaluations. The THEMIS code was generally used for the JEF-1 processing. In order to account for recent differential measurements and to improve the consistency between calculation and integral experiments, we produced our own CEA evaluations for the actinide nuclides : ^{235}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Am. This new APOLLO library was checked against critical experiments and PWR measurements : computed Conversion Factor, Reactivity Coefficients, Multiplication Factor, and Pu build-up are now in good agreement with LWR experimental results. PWR Pu recycling calculations, as does as HCLWR design studies, are also significantly improved.

(APOLLO Multigroup Library, JEF-1 file, CEA Evaluation, Integral Experiments).

I. INTRODUCTION

The feedback of PWR operation in the 900 MWe plants pointed out disagreements between measurements and core calculations : the computed negative moderator temperature coefficient was systematically overestimated in the start-up measurement / 1 / and spent fuel analyses / 2 / demonstrated discrepancies in the Pu build-up / 3 / and in the transactinide poisoning (Am and Cm isotopes). These trends derived from large PWR information were confirmed by specific experiments, respectively the CREOLE experiment / 4 / with isothermal temperature coefficient measurements in a pressurised loop, an the GEDEON irradiation / 5 / of a 15 x 15 UO_2 assembly at the centre of the MELUSINF 8 MW experimental reactor.

Moreover the large scale Pu recycling in the Electricité de France PWRs, induces new requirements on the reliability of MOX lattice calculations. Advanced PWRs design and HCLWR conception / 6 / noise additional needs on plutonium cross-section accuracy, particularly in the resonance energy range. Then, it became necessary to improve the APOLLO French assembly code / 10 / and to extend its application field :

- A new APOLLO library was processed from JEF-1 file and CEA internal evaluations ; this "CEA-86" multigroup library up-dates the "1979" previous recommended cross-section set.
- In order to compute PWR and HCPWR more accurately, improvements in self-shielding treatment were implemented in APOLLO and are extensively described in ref. / 7 / ; DOPPLER broadening and self shielding of epithermal resonances (E_R^{Pu0} = 1 eV ; E_R^{Pu2} = 2.67 eV) located below the APOLLO thermal cut-off are now automatically corrected by a fine mesh calculation, and an accurate resonance interaction model / 8, 9 / accounts for the mutual-shielding effect.

II. FILE PROCESSING AND CREATION OF MULTIGROUP CROSS-SECTIONS

The updated 99 groups library of the APOLLO spectrum code is based on the more recent nuclear data evaluations, particularly the JEF-1 Joint Evaluated File. We used generally the THEMIS Code to process these evaluation.

In the resonance range effective cross-section tabulations were computed by the AUTOSECOL Code / 11 / on an ultrafine optimized energy mesh. Reich and Moore formalism was used for ^{238}U and ^{239}Pu resonant cross-section rebuilding. In the unresolved resonance range, on improved ladder method was implemented : the "regularized pattern" / 12 /. The actual fine structure of the fuel flux is computed by AUTOSECOL without approximations on the slowing-down operator R_i of the resonnant isotope i :

$$(1/N_i).R_i\,\varphi(u) - (\sigma_{ti}(u) + \sigma_e).\,\varphi(u) + \sigma_e = 0$$

Then, effective multigroup cross-sections are pretabulated in the APOLLO library :

$$\sigma_{effi}^{K} = (1/\Delta u_g).\int_{\Delta u_g} \sigma_i^{K}(u).\ \varphi_i(u)\,du$$

where K = scattering, capture, fission.

These tabulations are defined for about 10 σ_e background cross-section values, and are temperature dependant.

This dependance of self-shielded cross-sections with temperature (^{235}U, ^{236}U, ^{238}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu and zirconium in the "CEA 86" library) enables APOLLO to account for DOPPLER effect with accuracy. Moreover, crystalline binding effect is accounted for a Debye temperature.

A Fission-Product cross-section set was processed / 13 / with the THEMIS code from the JEF-1 library.

New multigroup cross-section of Minor Actinides were defined in order to improve fuel cycle calculations : ^{232}U, ^{234}U, ^{236}Pu, ^{238}Pu and ^{243}Am JEF-1 files were processed and seemed satisfactory / 14 /.

III. FRENCH EVALUATIONS IN THE "CEA 86" LIBRARY

Even using the more recent nuclear data evaluations such as JEF-1 files, the correspondant multigroup cross-sections were not completely satisfactory compared to integral experiments and large PWR information.

Then we produced our own evaluations, specifically for the most important actinide nuclides : ^{235}U, ^{238}U, ^{239}Pu and ^{240}Pu. We used, in the one hand recent differential measurements in Geel and ORNL LINAC (post ENDF/BV and JEF-1 evaluations), and in the other hand French integral experiments / 15 /.

The spent fuel analyses / 2,3 / from FRAMATOME PWRs, and from the 15 * 15 UO_2 Gedeon assembly irradiated in the MELUSINE experimental reactor, enabled us to determine the right evaluation for capture and fission cross-section ; Conversion Ratio $\sigma_c\,^{238}U/\sigma_f\,^{235}U$ and Spectrum Index measurements ($\sigma_f\,^{8}U/\sigma_f\,^{5}U$, $\sigma_f\,^{9}Pu/\sigma_f\,^{5}U$, $\sigma_f\,^{0}Pu/\sigma_f\,^{9}Pu$, $\sigma_f\,^{1}Pu/\sigma_f\,^{9}Pu$,...) in the MINERVE and EOLE reactors were also used / 15, 16 /. The thermal cross-section shapes were modified in order to improve temperature reactivity coefficient calculation, particularly in the CREOLE experiment.

Then, a tendency research method / 24 / was applied on an exhaustive buckling measurement set, including French Pu tight-lattice investigation in the ERASME experiments / 16 / and also non LWR lattices ; the experimental data base involves Kinfinity, B^2m and M^2 measurements in LWR lattices with moderation ratio ranging from 0.45 to 5.5 (CRISTO / 17, 18 / and CAMELEON / 19 / French benchmark experiments). This study allowed us to calibrate the neutron multiplicity υ for the fissile nuclides in thermal and epithermal ranges.

III.1. ^{235}U nuclear data evaluation

In order to reduce the calculation - Experiment discrepancy in Reactivity Temperature Coefficient (RTC) measurements, we proposed new ^{235}U thermal cross-section shapes at the CHICAGO Conference in 1984 / 4 / ; instead of arbitrarily fitting the identified wrong data, we defined an evaluation of the thermal cross-sections based on the consideration of the basic nuclear data, i.e. the resonance parameters and the associated statistic laws : the procedure is detailed in a recent publication / 1 /.

In order to be closer from the 1/v law then the ENDF/BV evaluation, we used a more negative energy location (ΔE_R = - 0.25 eV compared to ENDF/BIV) of the first large bound level :

E_l^- = - 0.80 eV Γ_f = 230 meV

Γ_γ = 31 meV $g.\Gamma_n^\circ$ = 0.34

The corresponding fission cross-section was supported a posteriori by the ORNL measurements / 20 / and the Geel Linac results / 21 / in 1985 (see figure 1 below).

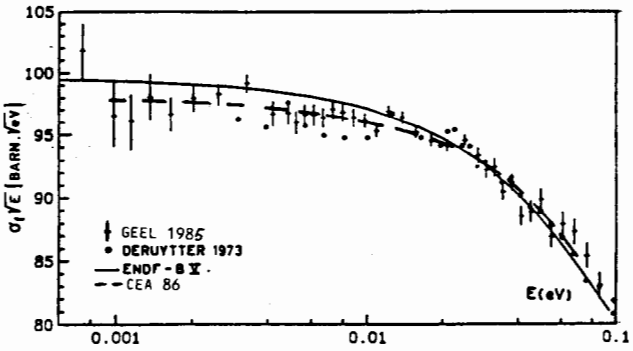

FIGURE 1 : ^{235}U FISSION CROSS-SECTION SHAPE

In order to obtain a more negative RTC component, we introduced a small negative "capture" resonance close to the zero energy :

Γ_γ = 40 meV Γ_f = 10 meV

$g.\Gamma_n^\circ = 1.6 \times 10^{-4}$ meV

Capture cross-section level was adjusted to a σ_c^{2200} = 99.2 b value to reproduce ^{236}U build-up in PWR lattices / 3 / ; the corresponding thermal σ_c^{235} cross-section was consistent with Gwin capture measurements inside the experimental uncertainty margins.

We adopted a $^{235}\nu$ flat shape ; the corresponding ν = 2.420 value was deduced from buckling measurements.

The resulting $^{235}\eta$ neutron yield per absorption is compared on figure 2 to the usual flate shape : this figure points out that our proposal was in agreement with the unique $^{235}\eta$ direct measurement from 1956 / 22 /.

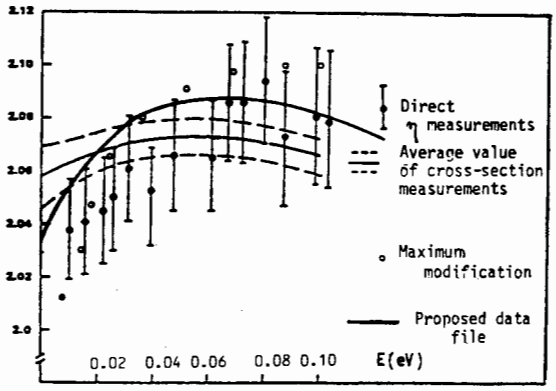

FIGURE 2 : FRENCH EVALUATION AND MEASUREMENTS OF η^{235}

Geel preliminary results of $^{235}\eta$ measurements for subthermal neutron energies were presented by Weigmann at the IAEA Advisory Group Meeting on Nuclear Data for RTC calculations (Vienna 7-10 December 1987) : Gelina linac results (including multiple scattering corrections), which are plotted on figure 3, confirm the CEA 86 cross-section set.

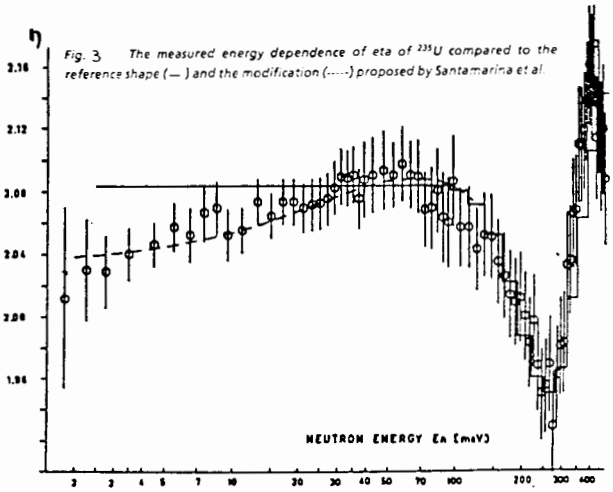

FIGURE 3 : $^{235}\eta$ GEEL MEASUREMENT AND CEA-86 LIBRARY

III.2. ^{238}U cross-section set

Accordingly to the recent 1977 measurements at Geel, ORNL and RPI, we used the Γ_γ = 23 meV De-Saussure evaluation / 23 / for the first three s-waves ; this low Γ_γ value, compared to the Γ_γ = 25-26 meV in ENDF/BIV, was consistent with ^{239}Pu build-up in large PWRs / 3 /.

In the upper part of the resonance range, (454 eV ; 3.36 KeV), the average capture cross-section was decreased compared to the ENDF/BV and JEF-1 values in order to improve the Calc.-Exp. comparison on σ_c ^{8}U/σ_f ^{5}U conversion ratio measurements in the ERASME tight lattices / 16 / :

σ_c (ENDF/BV) = 2.37 b

σ_c (JEF-1) = 2.32 b

σ_c (CEA 86) = 2.20 b

Effective cross-section tabulations were obtained in a Reich-Moore formalism : the increase of the self-shielding effect, due to modification of the scattering cross-sections, leads to a reactivity worth $\Delta K/K = -3 \times 10^{-3}$ in HCLWR lattices. In the unresolved range, more accurate self-shielded factors were obtained in the "regularized ladder method" / 12 / by random sampling of the energy levels and resonance parameters.

III.3. ^{239}Pu multigroup cross-sections

In the fast energy range and the resonance region, the JEF-1 file was used ; effective cross-section were computed in the Reich-Moore model. This multigroup library looked satisfactory in HCLWR benchmark experiments and in the voided ERASME configuration.

Below 3 eV, we needed to improve the Derrien evaluation and we produced an internal CEA evaluation based on French integral experiment :

- spent fuel analysis indicated that the "thermal" capture was slightly underestimated in the JEF-1 evaluation : we increased / 14 / the α value in the large E_R = 0.3 eV resonance, accordingly to the direct α ^{239}Pu measurements of Riabov / 25 /. In the "maxwellian" range we defined the α^{2200} = 0.365 and σ_c^{2200} = 273 barns normalization values,

- a non flat ν value was used. This is due to the n,γ_f and the spin effect on the nuclear energy dependance. The CEA 86 $\nu^{239}(E)$ is plotted on figure 4 : this shape is in agreement with the recent Gwin differential measurement and with theoretical studies / 26 /. Buckling measurements gave a trend in reducing $\nu(E)$ level and we adjusted the following value : ν^{2200} = 2.870 (compared to the ν^{2200} = 2.879 $\pm$ 0.006 Axton evaluation / 27 /).

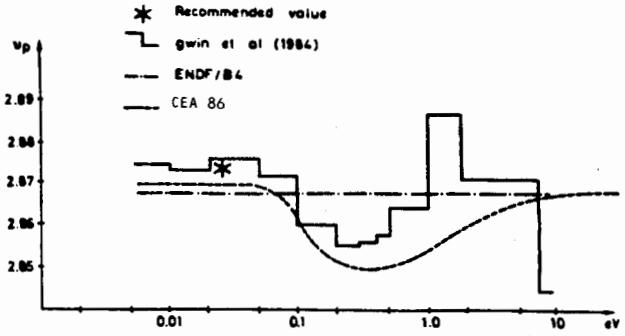

FIGURE 4 : $^{239}\nu$ SHAPE IN THE THERMAL RANGE

III.4. Minor Actinide cross-sections

- Internal evaluations were used for ^{236}U, ^{237}Np : corresponding multigroup APOLLO sets enables us to compute accurately ^{237}Np and ^{238}Pu build-up in PWR spent fuel analyses.

- We used the following parameters for the large ^{242}Pu resonance :

E_R = 2.67 eV $g.\Gamma_n$ = 2.00 Γ_γ = 25 meV

This trend was suggested by ^{242}Pu concentrations in high burn-up PWR assemblies (τ > 30 GWd/T) and by the initial ^{243}Am build-up.

- For ^{241}Am we adopted a high level in the thermal capture : σ_c^{2200} = 595 barns in agreement with the JEF-1 evaluation, and in the large resonance at E_R = 0.307 eV : Γ_γ = 47 meV, $g.\Gamma_n$ = 0.0283 meV ; the corresponding CEA 86 cross-sections are satisfactory for ^{242m}Am + ^{242}Cm build-up calculations ; recommanded branching ratios were derived from spent fuel analyses / 3 /.

IV. QUALIFICATION THROUGH INTEGRAL EXPERIMENTS

The APOLLO 1986 version was checked against an extensive set of integral experiments, including foreign benchmark experiments.

The reinterpretation of all isothermal Temperature Coefficient experiments has validated / 1 / these new cross-section. CREOLE (French benchmark RTC experiment with pressurised water up to 300°C / 4 /) interpretation calculations, with CEA 86 and with previous APOLLO library corresponding to standard thermal $\sigma^{235}U$ shape, are compared in table I : Calculation and Experiment are now in agreement within experimental uncertainty margins.

Temperature Range	$\alpha^{1979}_{calc} - \alpha_{meas}$	$\alpha^{1986}_{calc} - \alpha_{meas}$
20°C - 90°C	- 4.8 ± 2.0	- 1.7 ± 2.0
90°C - 190°C	- 2.6 ± 1.5	- 0.5 ± 1.5
190°C - 245°C	- 2.2 ± 1.5	- 0.7 ± 1.5
245°C - 290°C	- 2.1 ± 2.0	- 0.8 ± 2.0

TABLE I
CALCULATION - EXPERIMENT COMPARISON IN THE RTC CREOLE EXPERIMENT

($\Delta\alpha$ in 10^{-5} $\frac{\Delta K}{K}$/°C)

Spent fuel analyses in Tihange / 2 / and Fessenheim / 3 / 900 MWe PWR reactors demonstrated that Pu build-up is well reproduced by APOLLO-CEA 86 ; as an example, the C/E discrepancy shapes on ^{242}Pu concentration versus burn-up are graphed on figure 5 for the superseded 1979 version and with the APOLLO 1986 version. Figure 5 points out the improvement of our cross-section sets compared to ENDF/BV evaluations.

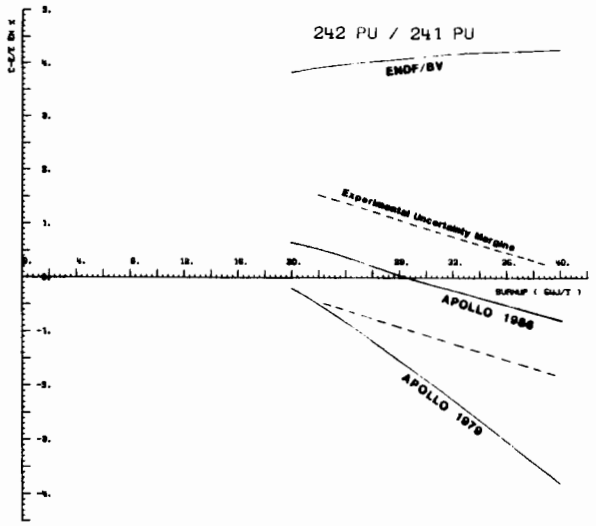

FIGURE 5 : ^{242}Pu BUILD-UP

Calculation of the GEDEON PWR assembly / 5 /, irradiated in the experimental MELUSINE reactor up to 10 GWd/T, supplied information at low burn-up : table II demonstrates the adequacy of actinide capture and fission cross-sections in the APOLLO library. The Calc./Exp. agreement on $^{239}Pu/^{238}U$ concentration ratio confirms that Conversion Ratio is accurately computed in PWR lattices.

Isotopic Ratio	$(C^{79}-E)/E$	$(C^{86}-E)/E$
$^{236}U/^{238}U$	- 0.6 ± 0.6 %	- 1.1 ± 0.6 %
$^{239}Pu/^{238}U$	- 0.9 ± 0.5 %	- 1.1 ± 0.5 %
$^{240}Pu/^{239}Pu$	- 1.4 ± 0.8 %	+ 0.8 ± 0.8 %
$^{241}Pu/^{240}Pu$	+ 1.7 ± 1.0 %	+ 0.3 ± 1.0 %
$^{242}Pu/^{241}Pu$	+ 3.3 ± 1.5 %	+ 2.2 ± 1.5 %

TABLE II
SPENT FUEL ANALYSES IN THE GEDEON EXPERIMENT
(average biases on three successive unloaded pins : 3 to 9 GWd/T)

Heavy nuclide component on the PWR reactivity loss per cycle is improved in the 1986 version. Nevertheless, the main improvement concerns minor actinide and fuel cycle calculations : the long standing disagreement / 28 / in ^{243}Am and ^{244}Cm build-up is worked out with CEA 86, as demonstrated by the Tihange spent fuel C/E comparison displayed on figure 6.

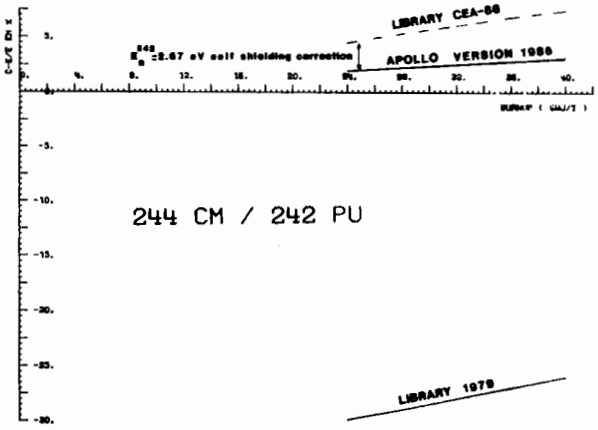

FIGURE 6 : $^{244}Cm/^{242}Pu$ C/E SMOOTHED SHAPE

Multiplication Factor calculation in Uranium fueled lattices is very satisfactory ; Figure 7 shows the Calc.-Exp. K_{eff} discrepancies for 35 buckling measurements in H_2O, D_2O and graphite moderators / 29 / : for well thermalized lattices with maxwellian spectrum, corresponding to a slowing -down density q > 0.7, the average C-E bias is cancelled ; figure 7 indicates that multiplication factors of PWR lattices (q ≅ 0.6) and of undermoderated water lattices are also accurately computed with APOLLO-CEA 86.

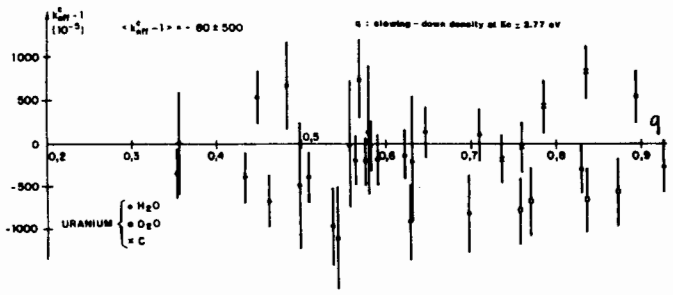

FIGURE 7 : K_{eff} C/E COMPARISON IN U LATTICES

Improvement in LWR K_{eff} calculation with APOLLO CEA-86 is confirmed by the French specific buckling measurements : APOLLO calculations are described in table III for 3 % ^{235}U enriched UO_2 fuel, used in the CRISTO experiments / 18 / (ten regular lattice configurations) and the CAMELEON PWR benchmark experiment / 19 /.

EXPERIMENT	CRISTO I	CRISTO II		CAMELEON
Ø in cm	1.86	1.71	1.58	1.26
V_{H_2O}/V_{UO_2}	5.46	4.40	3.56	1.79
$C^{1979} - E$ (10^{-5} ΔK/K)	+842	+587	+446	+977
$C^{1986} - E$ (10^{-5} ΔK/K)	+371	+91	-15	+570
$\Delta K_{eff}^{exp}(1\sigma)$	±310	±240	±330	±220

TABLE III
APOLLO CALCULATION OF LWR BUCKLING MEASUREMENTS IN EOLE REACTOR

Major improvements due to the CEA-86 library arises in Pu fueled lattices ; APOLLO-86 calculations of multiplication factor in French Pu critical experiments are plotted on figure 8 : Keff of MOX assemblies in PWR Pu recycling, corresponding to q = 0.5 - 0.6 slowing-down density range, are perfectly adjusted. Multiplication factors of HCLWR tight lattices are now well reproduced, as demonstrated in figure 8 by the ERASME "S" and ERASME "R" experiments / 16 /.

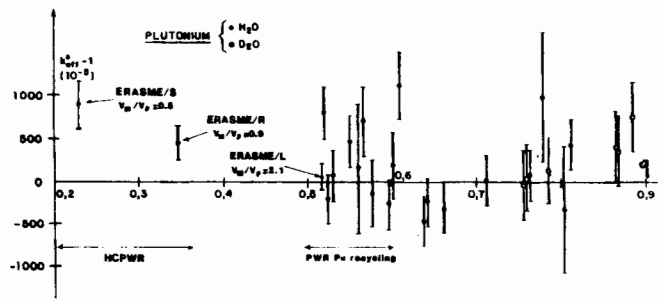

FIGURE 8 : APOLLO CEA-86 MULTIPLICATION FACTOR OF Pu FUELED LATTICES

V. SUMMARY

The new APOLLO version and its "CEA 86" multigroup library, based on JEF-1 file and on our own CEA evaluations, is operating since March 1986 in PWR and HCR calculations.

This new library was checked against critical experiments and PWR measurements : computed Conversion Factor, Reactivity Coefficients, Multiplication Factor and Pu build-up are now in good agreement with LWR experimental results. PWR Pu recycling calculations, as does as HCPWR design studies, are also significantly improved.

REFERENCES

/ 1 / A. SANTAMARINA - IAEA Advisory Group Meeting of Reactiv. Coeff. Calc. VIENNE 7-11 Dec. 1987.
/ 2 / P. GAUCHER, L. MARTIN-DEIDIER, A. SANTAMARINA et al. Proc. ANS. Top. Meet. React. Phys. 1, 56 CHICAGO (1984).
/ 3 / P. GAUCHER, A. SANTAMARINA - Proc. ANS Top. Meet. React. Phys. 1, 457, SARATOGA 1986).
/ 4 / A. SANTAMARINA et al. Proc. ANS Top. Meet. React. Phys. 1, 48 CHICAGO (1984).
/ 5 / P. CHAUCHEPRAT, A. SANTAMARINA Proc. Int. Top. Meet. React. Phys. & Math., 1, 199 PARIS (1987).
/ 6 / B. BARRE, M. DARROUZET et al. ENC-4, GENOVA 86.
/ 7 / A. SANTAMARINA et al. HCLWR Group. Meet. NEA-Data bank SACLAY (Avril 1988).
/ 8 / A. SANTAMARINA - Annals of Nucl. En., 3, p 1-9 (1976).
/ 9 / B. GASTALDI - Ph. D. Thesis - ORSAY (10 July 86).
/ 10 / A. KAVENOKY et al, 3, PARIS (27-30 april 87).
/ 11 / M. GRANDOTTO - Ph. D Thesis - ORSAY (1974).
/ 12 / P. RIBON, CEA-N-2426 Report (1985).
/ 13 / J. KREBS - Private communication (1986).
/ 14 / A. SANTAMARINA - JEF/Doc-182, SACLAY (12 May 87).
/ 15 / A. SANTAMARINA, M. DARROUZET, L. MARTIN-DEIDIER - Proc. Int. Conf. Nucl. Data, 1 509 SANTA FE (1985).
/ 16 / L. MARTIN-DEIDIER, A. SANTAMARINA, S. CATHALAV et al., Proc. Meet. React. Phys., 1 97, PARIS (1987).
/ 17 / A. SANTAMARINA - 24 th NEACRP Meeting (1982).
/ 18 / A. SANTAMARINA - Proc. ANS Top. Meet. Phys. 1, 937 (1982).
/ 19 / L. MARTIN-DEIDIER, A. SANTAMARINA et al. Trans. ANS, 46, 755 (1984).
/ 20 / R. GWIN et al - Nucl. Sci. Eng., 88, 37 (1984).
/ 21 / WAGEMANS, DERUYTTER - SANTA FE, 1 499 (1985).
/ 22 / PALEVSKY et al., J. Nucl. Energy, 1, 177 (1956).
/ 23 / G. DE SAUSSURE et al. Progress in Nucl. En., 3 87 (79).
/ 24 / P. REUSS - Note CEA N2222 (1981).
/ 25 / J.V. RIABOV - AE 41, 1, 45 (1976).
/ 26 / E. FORT et al., To be presented at this conf.
/ 27 / E.J. AXTON, Report CBNM GE/PH/01/86 (1986).
/ 28 / J. BOUCHARD et al. Proc. ANS Top. Meet. Phys. SUN VALLEY (82).
/ 29 / H. TELLIER et al. Proc. SARATOGA, 1, 419 (1986).