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STATUS OF THE PU239 EVALUATION IN THE RESONANCE RANGE FOR JEFF

CONTRIBUTIONS FROM CEA/DEN CADARACHE

Gilles NOGUERE

CM-INDEN on the resonance parameters of actinides IAEA, 8-11 may 2018

www.cea.fr

Ces

JEFF-3.1.1

- Good performances of the JEFF-3.1.1 library on PST benchmarks
- However, several physical problems still unsolved

JEFF-3.2

- Improved MOX calculations, mainly due to new Am241 evaluation
- Pu239 evaluation comes from WPEC/SG34
 - \Rightarrow 3 resolved resonance ranges are merged
 - \Rightarrow good performances on PST are preserved
 - \Rightarrow Resonance Parameter Covariance Matrix is given

JEFF-3.3

- New Pu239 resonance parameters (to solve some missing interferences, ...)
- Upper energy limit of the RRR is increased up to 4.5 keV

JEFF-x.x

- New PFNS
- New Thermal Neutron Constants
- New modeling of the fission process: Include $(n,\gamma f)$ reaction, add class II states ...

Solve inconsisent RTC results with measurements performed in the EOLE reactor

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Pu239 evaluation in JEFF-3.1.1

Resonance range divided into three resonance parameter sets (computer limitations)



Background cross section (for fission) not used in the resolved resonance range of JEFF-3.1.1





Modification of α (Pu239) in JEFF-3;1;1 to improve the reactivity temperature coefficient (RTC) in EOLE experiments, cold conditions 20-80°C (JEF/DOC-1158)



Pu239 evaluation in JEFF-3.1.1



TABLE XIX: The average values for C/E - 1 (in pcm) for ENDF/B-VII.1 per main ICSBEP benchmark category.

		COI	MP			M	EΤ		SOL	MIX	ED
	therm	inter	fast	mixed	therm	inter	fast	mixed	therm	therm	fast
LEU	J -80				553				133		
IEU	J 101	-253	-70				103		396		
HEU	J 746	2112		-892	130	-65	114	844	16		
MD	X 402		16				418		-194	322	-845
PU	J	1119		1960		2950	164	921	462		
U23	3 23						-220		549		

TABLE XX: The average values for C/E - 1 (in pcm) for JENDL-4.0 per main ICSBEP benchmark category.

		-									
		CO	MP			M	ET		SOL	MIX	ED
	therm	inter	fast	mixed	therm	inter	fast	mixed	therm	therm	fast
LEU	-29				736				-90		
IEU	87	-257	-209				-435		487		
HEU	985	2982		-497	397	209	31	948	197		
MIX	501		446				194		16	588	-591
PU		1376		2030		3529	0	970	633)	
U233	25						-195		177		

good performances of the JEFF library on PST benchmarks

TABLE XXI: The average values for C/E - 1 (in pcm) for JEFF-3.1.1 per main ICSBEP benchmark category.

		COI	MP			Μ	ΕT		SOL	MIX	ED
	therm	inter	fast	mixed	therm	inter	fast	mixed	therm	therm	fast
LEU	-52				527				179		
IEU	-107	-468	258				-180		425		
HEU	381	1912		-1221	-45	145	-106	628	-56		
MIX	258		300				251		-274	87	-867
PU		692		1852		3275	95	478	203)	
U233	-312						363		22.7		

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Pu239 evaluation in JEFF-3.2



WPEC/SG34 \Rightarrow the non-regression of the Pu239 nuclear data was continuously monitored during the evaluation procedure with a selected set of ICSBEP benchmakrs

Crucial step to conserve the good performances of the JEFF library on PST benchmarks

TABLE XIX: The average values for C/E - 1 (in pcm) for ENDF/B-VII.1 per main ICSBEP benchmark category.

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PU		692		1852		3275	95	478	203)	
U233	-312						363		237		



Pu239 evaluation in JEFF-3.2



JEFF-311 and JEFF-32 \Rightarrow Similar results for Plutonium in THERM spectrum

PAGE 10

Integral experiments carried out in the EOLE reactor of CEA Cadarache Interpretation with the Monte-Carlo and deterministic codes TRIPOLI, MVP and APOLLO



Average value obtained with JEFF-32 \Rightarrow (C-E)=+50 pcm with a standard deviation of 180 pcm



CERES program (P. Leconte, PHYSOR 2014)

- Collaboration between Winfrith and Cadarache (1992-1995) as part of the CEA/UKAEA collaboration on LWRs
- Experiments conducted in the DIMPLE (AEA) and MINERVE (CEA) reactors on common samples, manufactured both at Cadarache and Winfrith
- Reactivity-worth measurements of fresh MOX fuel samples provided by CEA and AEA





Integral results for $v\Sigma_f$ (SG-34)

@ P. Leconte

Reactivity breakdown (TOT=100)							
239	Σ_{a}	-9.0					
Pu	$\nu \Sigma_{f}$	98.5					
²⁴⁰ Pu	Σ_{a}	-0.9					
241	Σa	-1.0					
Pu	$\nu \Sigma_f$	12.3					

Reactivity breakdown (TOT=100)

239	Σ_{a}	-17.8
Pu	$\nu\Sigma_{f}$	118.0
²⁴⁰ Pu	$\Sigma_{\rm a}$	-0.3
241p.	Σ_{a}	
Pu	$\nu\Sigma_{f}$	0.1

	Ful	Monte Carlo	Method C/E-1	(%)
Sample (Reference)	Assembly-I	Assembly-II	Assembly-III	R1UO2
MOX1 (CEAU11)	3.0 ± 4.9	3.6 ± 9.3	10.9 ± 6.6	197 ± 9274
MOX2 (CEAU11)	0.7 ± 3.2	34.2 ± 22.8	5.7 ± 4.0	-59.2 ± 6.1
MOX3 (CEAU11)	0.8 ± 1.7	18.2 ± 4.8	2.9 ± 1.8	-79.6 ± 7.4
MOX4 (CEAU11)	-0.7 ± 1.5	9.6 ± 2.9	0.1 ± 1.3	-98 ± 8.7
MOX5 (CEAU11)	-1.1 ± 1.3	5.1 ± 1.5	-1.3 ± 1.1	97 ± 13.2
MOX6 (CEAU11)	-1.5 ± 1.2	1.4 ± 1.2		42 ± 7.8
Pu0403 (UO2nat)	-2.4 ± 1.5	-1.1 ± 4.0	-2.9 ± 2.4	-7.1 ± 4.5
Pu0413 (UO2nat)	-2.9 ± 1.7	-7.6 ± 6.8	-5.6 ± 2.6	-21.3 ± 10.2
Pu0426 (UO2nat)	-6.6 ± 1.6	-23 ± 5044	-8.1 ± 3.1	-93 ± 154
Pu2003 (UO2nat)	1.1 ± 1.4	0.1 ± 1.5	-0.7 ± 1.3	-7.7 ± 2.5
Pu2013 (UO2nat)	0.4 ± 1.4	3.0 + 2.0	-0.8 ± 1.3	1.7 ± 3.9
Pu2026 (UO2nat)	1.1 ± 1.4	22.4 ± 5.1	2.1 ± 1.5	-140 ± 22

Reactivity breakdown (TOT=100)

239 _{D11}	Σ_{a}	-17.9
Pu	$\nu\Sigma_{f}$	118.7
²⁴⁰ Pu	Σ_{a}	-2.1
241	Σ_{a}	-0.3
Pu	$\nu \Sigma_{f}$	2.0

Mean value = -1.0 ± 0.5 % (standard deviation : 2.5%)



Integral results for K1 (SG-34)

Reactivity breakdown	
(TOT=100)	

239	Σ_{a}	-88.2
Pu	$\nu \Sigma_{f}$	185.5
²⁴⁰ Pu	Σa	-7.9
241	Σ_{a}	-10.3
Pu	$\nu \Sigma_f$	23.5

	Full Monte Carlo Method C/E-1 (%)							
ample (Reference)	Assembly-I	Assembly-II	Assembly-III	R1UO2				
MOX1 (CEAU11)	3.0 ± 4.9	3.6 ± 9.3	10.9 ± 6.6	197 ± 9274				
MOX2 (CEAU11)	0.7 ± 3.2	34.2 ± 22.8	5.7 ± 4.0	-59.2 ± 6.1				
MOX3 (CEAU11)	0.8 ± 1.7	18.2 ± 4.8	2.9 ± 1.8	-79.6 ± 7.4				
MOX4 (CEAU11)	-0.7 ± 1.5	9.6 ± 2.9	0.1 ± 1.3	-98 ± 8.7				
MOX5 (CEAU11)	-1.1 ± 1.3	5.1 ± 1.5	-1.3 ± 1.1	97 ± 13.2				
MOX6 (CEAU11)	-1.5 ± 1.2	1.4 ± 1.2		42 ± 7.8				
Pu0403 (UO2nat)	-2.4 ± 1.5	-1.1 ± 4.0	-2.9 ± 2.4	-7.1 ± 4.5				
Pu0413 (UO2nat)	-2.9 ± 1.7	-7.6 ± 6.8	-5.6 ± 2.6	-21.3 ± 10.2				
Pu0426 (UO2nat)	-6.6 ± 1.6	-23 ± 5044	-8.1 ± 3.1	-93 ± 154				
Pu2003 (UO2nat)	1.1 ± 1.4	0.1 ± 1.5	-0.7 ± 1.3	-7.7 ± 2.5				
Pu2013 (UO2nat)	0.4 ± 1.4	3.0 ± 2.0	-0.8 ± 1.3	1.7 ± 3.9				
Pu2026 (UO2nat)	1.1 ± 1.4	22.4 ± 5.1	2.1 ± 1.5	-140 ± 22				

Reactivity breakdown (TOT=100)

@ P. Leconte

	-	-
239 _{D.1}	Σ_{a}	-100.8
Pu	$\nu \Sigma_{f}$	202.4
²⁴⁰ Pu	Σ_{a}	-1.6
241	Σ_{a}	
Pu	$\nu \Sigma_{f}$	0.1

Reactivity breakdown							
	(TOT=100)						
239	Σ_{a}	-113.6					
Pu	$\nu \Sigma_{f}$	228.2					
²⁴⁰ Pu	Σ_{a}	-13.9					
241	Σ_{a}	-1.8					
Pu	$\nu \Sigma_f$	3.8					



Mean value = -0.4 ± 0.5 % (standard deviation : 5.2%)

Pu239 evaluation in JEFF-3.2

Propagation of the Pu239 resonance parameter uncertainties on EOLE benchmarks



Pu239 evaluation in JEFF-3.2

Propagation of the Pu239 resonance parameter uncertainties on EOLE benchmarks



Significant reduction of the Pu239 capture cross section uncertainties at low neutron energy





Pu239 evaluation in JEFF-3.2

No modification of the Pu239 fission cross section uncertainties







Final uncertainties after the Integral Data Assimilation of the CERES program

		Relative u	ncertainty		
	JEFF-3.2 (=3G34)	JEFF-3.2	COMAC-V2		
$\sigma_{\rm f}$	747.2 barns	0.9%	0.7%		
σγ	270.1 barns	4.4%	1.6%		
I _f	308.8 barns	2.3%	2.3%		
Ι _γ	180.1 barns	5.7%	5.7%		
K1	1161.5 barns	1.7%	0.9%		





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Improved Mixed Oxide Fuel Calculations with the Evaluated Nuclear Data Library JEFF-3.2

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> Abstract — An overestimation of the k_{eff} values for mixed oxide (MOX) fuels was identified with Monte Carlo (TRIPOLI-4) and deterministic (APOLLO2) calculations based on the Joint Evaluated Fission and Fusion (JEFF) evaluated nuclear data library. The overestimation becomes sizeable with Pu aging, reaching a reactivity change of $\Delta \rho \approx +700$ pcm for integral measurements carried out with MOX fuel containing a large amount of americium. This bias was observed for various critical configurations performed in the zeropower reactor EOLE of the Commissariat à l'énergie atomique et aux énergies alternatives (CEA), Cadarache, France. The present work focuses on the improvements achieved with the new ²³⁹Pu and ²⁴¹Am evaluated nuclear data files available in the latest version of the JEFF library (JEFF-3.2). The resolved resonance range of the plutonium evaluation was reevaluated at Oak Ridge National Laboratory (ORNL), Oak Ridge, Tennessee, with the SAMMY code in collaboration with CEA Cadarache. The resonance parameters of the americium evaluation were obtained with the REFIT code in collaboration with the research institutes Institute for Reference Materials and Measurements (IRMM), Geel, Belgium, and Institut de recherche sur les lois fondamentales de l'Univers (Irfu), Saclay, France.

Keywords — EOLE, MINERVE, TRIPOLI-4.

Cez

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- Upper energy limit of the RRR is increased up to 4.5 keV

JEFF-x.x

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- New Thermal Neutron Constants
- New modeling of the fission process: Include $(n,\gamma f)$ reaction, add class II states ...

Solve inconsisent RTC results with measurements performed in the EOLE reactor





Fluctuations observed in JEFF-311 \Rightarrow confirmed by Tovesson data (2010, LANL)



New capture data from Shea Mosby provide crucial trends to extend the RRR



Data from Mosby are shape data \Rightarrow A good agreement is obtained with the data from Gwin (normalisation with the PROFIL experiments carried out in the PHENIX reactor of CEA Marcoule) | PAGE 23

Optimization of resonance ladders randomly generated by using URR parameters from JEFF-311





Comparison with GMA/CONRAD results



Extension of the RRR from 2.5 keV to 5 keV in good agreement with the GMA analysis (differences of 4%)

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Impact of the extension of the RRR up to 5 keV



Significant impact (\approx 200 pcm) on SNEAK7A and SNEAK7B \Rightarrow sodium free configurations

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Impact of the mean neutron energy uncertainty on PST calculations

Y. Peneliau et al., Pu239 Prompt Fission Neutron Spectra Impact on a Set of Criticality and Experimental Reactor Benchmarks, ND2013 (2013)

Authors	years	$\langle E \rangle$	$\Delta[\langle E(PFNS) \rangle, \langle E(JEFF-32) \rangle]$	Δ [keff(PFNS),keff(JEFF-32)
N. Kornilov	2008	2,055	-2,8%	+680 pcm
L. Berge	2014	2,087	-1,2%	+316 pcm
V. Maslov	2008	2,092	-1,0%	+250 pcm
JEFF-32	2013	2,113	0%	0 pcm
P. Romano	2014	2,122	+0,4%	-90 pcm
O. Serot	2013	2,140	+1,3%	-290 pcm
D. Rochman	2014	2,195	+3,9%	-890 pcm

Uncertainty suggested by R. capote $\Rightarrow \Delta \langle E \rangle = \pm 1.5\% \Rightarrow \Delta \text{keff(PST)} \approx \pm 300 \text{ pcm}$



Impact of the mean neutron energy uncertainty on MOX fuel calculations



mean neutron energy uncertainty \Rightarrow low impact on EOLE benchmarks

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Determination of the TNC with the CONRAD code by using "mic" data from Axton

			AGS			Monte-Carlo (N=1000)			STD2018	
Therm constai	al nts	Values and fitting uncertainties Final unc.		Values and fitting uncertainties		Final unc.	Values	Final Unc.		
	$\sigma_{\rm s}$	7.99	(12.40%)	12.40%	7.99	(12.40%)	12.38%	7.8	12.82%	✓
D., 220	$\sigma_{\rm f}$	749.10	(0.35%)	0.45%	749.50	(0.27%)	0.49%	752.4	0.29%	×
Pu239	σ_{γ}	270.60	(1.02%)	1.07%	270.10	(0.91%)	1.15%	269.8	0.93%	✓
	υ_t	2.882	(0.19%)	0.20%	2.881	(0.13%)	0.23%	2.878	0.45%	×

 \Rightarrow CONRAD and GMA analysis provide similar results

Fission cross section uncertainty seems to be underestimated

 υ_t uncertainty seems to be overerestimated

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	JEFF-3.2	Relative uncertainty				
	(=SG34)	JEFF-3.2	COMAC-V2			
$\sigma_{\rm f}$	747.2 barns	0.9%	0.7%			
σ_{γ}	270.1 barns	4.4%	1.6%			
υ_t	2.875	-	0.1%			

Two problems in JEFF3.2 and COMAC-V2

- Fission cross section
- υ_t Uncertainty

Determination of the Westcott factors by using the "mac" data

Westcott factors were extracted from the macroscopic data of Axton by considering the TNC as fixed parameters with known uncertainties. Their uncertainties were propagated via the marginalization technique implemented in the CONRAD code.

		AGS Values and fitting uncertainties Final unc.			Monte-Carlo (N=1000)			[car09]		
Therm consta	nal nts			Final unc.	Values and fitting uncertainties		Final unc.	Values	Final Unc.	
D 11220	g a	1.079	(0.51%)	0.71%	1.081	(0.44%)	0.75%	1.078	0.22%	✓
Fuzos	g _f	1.053	(0.44%)	0.64%	1.053	(0.35%)	0.64%	1.055	0.21%	✓

	JEFF-3.2 (=SG34)
g _a	1,077
9 _f	1,052

Westcott factors in JEFF-3.2 \Rightarrow Ok

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Reich-Moore analysis with the CONRAD code



- New transmission of the 1st resonance is needed \Rightarrow Bollinger 1958 !!!
- Fission cross section ⇒ problems to normalize the 3 data sets from Weston
- Capture cross section ⇒ problems to normalize the capture data from Brooks (1966) and the 2 data sets from Gwin (1971)
- Mosby data not yet available
- Comparison with the Pu239 evaluation study of M. Alrwashdeh (ANE 118, 313, 2018)

"The R-Matrix formalism"

@ E. Leal Cidoncha





The observed fission is the sum of the « direct » fission and of the two-step (n, γ f) reaction:

 $\sigma_{f,obs}(E) = \sigma_{(n,f)}(E) + \sigma_{(n,\gamma f)}(E)$

Channel widths for the direct fission (n,f) and for the two-step (n, γ f) reaction

- Two openened fission channels for $J^{\pi}=0^+ \Rightarrow \Gamma_{f1}(0^+)$ and $\Gamma_{f2}(0^+)$
- One openened fission channels for $J^{\pi}=1^+ \Rightarrow \Gamma_f(1^+)$
- Two J-dependent widths for the (n, γ f) reaction $\Rightarrow \Gamma_{\gamma f}(0^+)$ and $\Gamma_{\gamma f}(1^+)$



Good agreement is obtained between the $(n,\gamma f)$ reaction deduced from the RRR and the AVXSF calculations (LANL/CEA collaboration)



The smallest resonances with $J^{\pi}=1^{+}$ are dominated by the (n, γ f) process

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New resonance analysis by including the (n, γ f) process

CONRAD analysis with the $(n,\gamma f)$ contribution



Strong impact \Rightarrow interferences between the resonances

Slight modification of the radiation widths (0.5 meV in average)



Behavior of the cross section between the resonance can be changed by using the imaginary part of the distant level parameter R^{∞}





Channel widths for the direct fission (n,f) and for the two step (n, γ f) reaction

- Two openened fission channels for $J^{\pi}=0^+ \Rightarrow \Gamma_{f1}(0^+)$ and $\Gamma_{f2}(0^+) \Rightarrow \Gamma_{f}(0^+)$
- One openened fission channels for $J^{\pi}=1^+ \Rightarrow \Gamma_f(1^+)$
- Two J-dependent widths for the $(n,\gamma f)$ reaction $\Rightarrow \Gamma_{\gamma f}(0^{+})$ and $\Gamma_{\gamma f}(1^{+})$

Four partial widths are introduced in the phenomenological description of υ_p

$$\upsilon_p(E) \approx \sum_{i=1}^4 \nu_i P_i(E) \qquad P_i(E) = \frac{\sigma_i(E)}{\sigma_{(n,f)}(E) + \sigma_{(n,f)}(E)}$$



Contribution of the (n, γ f) process can be observed for resonances with J^{π}=1⁺



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 \Rightarrow Consistent description of the phase shift and neutron penetration factor

Cea

Evolution of the JEFF library for MOX fuel calculations

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Integral validation with EOLE experiments as a function of the temperature (CEA Cadarache)

