- Infu





The NEVFAR project:

New Evaluation of v Fluxes At Reactors

DE LA RECHERCHE À L'INDUSTRIE



Revisiting the summation calculation of reactor antineutrino spectra

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IAEA TM on Nuclear Data Needs for Antineutrino Spectra Applications 18 January 2023

www.cea.fr

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OUTLINE

1. Introduction & motivations

- a. Reactors as antineutrino sources
- b. Experimental anomalies
- c. Different modeling methods

2. Revised summation method

- a. β^{-} spectrum calculation
- b. Nuclear data content
- c. Uncertainty budget

3. Preliminary comparisons

- a. Integral measurements
- b. Spectrum shape

4. Conclusion & perspectives



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PRESSURIZED WATER REACTOR (PWR)

- Fuel: lowly enriched uranium, ²³⁸U + 3-5% ²³⁵U
- High power: ~3 4 GW_{th}

BD threshold

Reactor v spectrum [v/MeV/fission]

Similar reactor design & fuel contents for all PWR

\Rightarrow Similar \bar{v}_{e} spectra

RESEARCH REACTOR

- Fuel: highly enriched uranium, >20% ²³⁵U
- Low power : ~0.1 kW_{th} 100 MW_{th} but very short baseline accessible
- Wide array of designs & fuel contents + reactor specific structural material activation

\Rightarrow Reactor-specific $\bar{\nu}_{e}$ spectra



 $\Rightarrow \bar{\nu}_{\rho}$ contribution depends on reactor type and changes with time

⇒ Prediction needed for fission and activation spectra

REACTOR ANTINEUTRINO ANOMALY (RAA)

- Systematic IBD rate deficit vs to HM
- Measured/predicted IBD rate: **0**. **936**^{+0.024}_{-0.023} (2.5σ)
- RAA possible origins
 - Experimental bias

- Unlikely
- New physics (sterile neutrino)
- \blacktriangleright Mismodeling / underestimation of $\overline{\nu}_e$ spectrum uncertainty
- Single / multiple actinide(s) ?



SHAPE ANOMALY

- First observed by Double Chooz, Daya Bay; RENO
 - Confirmed by recent very-short baseline reactor exp. (NEOS, STEREO, PROSPECT, DANSS)
- Possible origins
 - Detector energy scale calibration
 Checked
 - Fuel composition
 - Prediction issue, single / multiple actinide(s) ?

FUEL-DEPENDENT IBD RATE EVOLUTION

- IBD yield changes with fuel evolution of PWR
- Comparison between measured IBD yield evolution and predicted evolution
 - 3.1σ at Daya Bay
 - 1.3σ at RENO
- Induced by inequal fractional deficit among actinides







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1. Introduction & motivations

REACTOR DATA-DRIVEN METHOD

- Unfolding exp. prompt IBD spectrum
 - $\triangleright \bar{\nu}_e$ spectrum + covariance matrix

PROS 🚽

- Model-independent (no anomalies)
- Small uncertainties

- Limited to exp. range, 1.8-9 MeV
- Small number of available datasets
- No activation spectrum



c. Different modeling methods

CONVERSION METHOD

- Measure exp. β fission spectra
- Convert virtual β branch fit to $\bar{\nu}_e$ branches

沟 PROS

- Small uncertainties ~2-3%
- Access total \bar{v}_e fission spectrum

- Limited to exp. range, 2-8 MeV
- No activation spectrum
- HM subject to the anomalies
- BILL data questionned \rightarrow KI exp.
- Impact of forbidden branches on fit



SUMMATION METHOD

- Fission spectrum prediction = sum of all β branches listed in nuclear databases
- +900 β^- emitters ~ 10 000 β^- transitions

沟 PROS

- Prediction ∀ energy, ∀ β emitter
 CEvNS
- Convenient to understand physics
- Mandatory for activation spectra

- Uncomplete/biased nuclear database
- Modeling approximations
- · Uncertainties very complex to estimate



1. Introduction & motivations

REACTOR DATA-DRIVEN METHOD

- Unfolding exp. prompt IBD spectrum
 - $\triangleright \bar{\nu}_e$ spectrum + covariance matrix

PROS 🚽

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- Small uncertainties

E CONS

- Limited to exp. range, 1.8-9 MeV
- Small number of available datasets
- No activation spectrum

Daya Bay: Total, ²³⁵U, ²³⁹Pu RENO, NEOS: Total

STEREO, PROSPECT: ²³⁵U

c. Different modeling methods

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- · Uncertainties very complex to estimate

Huber-Mueller model (+ KI data)

⇒ ²³⁵U, ²³⁹Pu and ²⁴¹Pu from P. Huber PRC 84, 024617 (2011)

 $\Rightarrow \frac{^{235}\text{U}/^{239}\text{Pu data from Kl}}{^{\text{PRD 104, L071301 (2021)}}}$

⇒ ²³⁸U from Mueller *et al.* PRC 83, 054615 (2011)

c. Different modeling methods

THE NEvFAR PROJECT

(New Evaluation of v Fluxes At Reactor)



- Revise summation method with BESTIOLE code
 - ightarrow Improve β -decay modeling
 - Refine non-unique forbidden transition modeling
 - Impact of database uncompleteness and quality
 - Update nuclear database with Pandemonium-free data
 - Adjusted effective modeling for nuclides with no data
 - Build a comprehensive uncertainty budget
 - Nuclear data and modeling uncertainties



SUMMATION METHOD

- Fission spectrum prediction = sum of all β branches listed in nuclear databases
- +900 β^- emitters \sim 10 000 β^- transitions

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- Prediction ∀ energy, ∀ β emitter
 ► CEvNS
- Convenient to understand physics
- · Mandatory for activation spectra

- Uncomplete/biased nuclear database
- Modeling approximations
- Uncertainties very complex to estimate

⇒ Reliable summation method required for multiple purposes



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W. Bühring and H. Behrens formalism (1982)



- W: β total energy
- W₀: max available energy
- $E_0 = W_0 m_e$: max kinetic energy
- K: normalization factor $\int dW S_{\beta} = 1$

$$S_{\beta}(Z, A, W) = K \frac{pW(W_0 - W)^2}{F_0(Z, A, W)} C(Z, A, W) (1 + \delta_{WM} + \delta_{RC})$$

V-A THEORY OF β -DECAY

- Phase space
 - \triangleright Energy states accessible to the emitted β
- Fermi function
 - \triangleright Electromagnetic interaction β / daughter nucleus
 - \triangleright Depends on β wavefunction
- Shape factor
 - ▷ Nuclear structure effect, depends on spin-parity
 - \triangleright Depends on β wavefunction



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V-A THEORY OF β -DECAY

• Phase space

ightarrow Energy states accessible to the emitted β

Fermi function

- \triangleright Electromagnetic interaction β / daughter nucleus
- \succ Depends on β wavefunction

Shape factor

- Nuclear structure effect, depends on spin-parity
- Depends on β wavefunction

Behrens & Bürhing algorithm (1982)

- $\checkmark\beta$ wavefunction computation depends on nuclear potential
- ✓ Reproduce Berhens & Jänecke tables
 - Finite-size and screening corrections to Fermi functions and to unique forbidden shape factors
- ✓ Extended to any energy, for any spherical nuclear potential



⇒ Impact of more realistic nuclear potential modeling <0.2% on fission spectrum shape and IBD yield</p> W. Bühring and H. Behrens formalism (1982)

a. β^{-} spectrum calculation

• *p*: β momenum

- *W*: β total energy
- W₀: max available energy
- $E_0 = W_0 m_e$: max kinetic energy
- *K*: normalization factor $\int dW S_{\beta} = 1$

e, E_=10

--- e⁻, E_v=1.8

- v, E₄=10

···· ν, Ε =1.8

0.8 1 Normalized kinetic energy

$$S_{\beta}(Z, A, W) = K \, p W(W_0 - W)^2 \, F_0(Z, A, W) \, C(Z, A, W) \, (1 + \delta_{WM} + \delta_{RC})$$

V-A THEORY OF β -DECAY

- Phase space
 - \triangleright Energy states accessible to the emitted β
- Fermi function
 - \triangleright Electromagnetic interaction β / daughter nucleus
 - \succ Depends on β wavefunction
- Shape factor
 - Nuclear structure effect, depends on spin-parity
 - \succ Depends on β wavefunction
- Radiative correction (RC)
 - ▷ QED effect from virtual photon exchange
 - $\, \vartriangleright \, \beta \, \text{correction} \gg \bar{\nu}_e \, \text{correction}$
- Weak magnetism correction (WM)
 - ▷ Nucleon structure effect
 - ▷ Depends on spin-parity info





0.6

0.4

WM correction in Behrens & Bürhing \rightarrow allowed GT and non-unique forbidden

- ✓ Apply WM correction of allowed GT to non-unique forbidden branches
- ✓ Uncertainty derived for fission spectra → $\sigma_{IBD}(WM) = 0.3\%$

CLASSIFICATION OF β^- TRANSITIONS

Fluxes for typical PWR fission fractions

β -decay type	ΔJ	$\pi_i \pi_j$	Shape factor	Calculation	ν̄ _e [%]	IBD [%]
Allowed	0,1	+1	1	Debuet and example	61	47
Unique forbidden	n + 1	$(-1)^{n}$	Polynomial in $p_v \& p_e$	Robust and accurate	10	9

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Allowed	0,1	+1	1	Debuct and ecourate	61	47
Unique forbidden	n + 1	$(-1)^{n}$	Polynomial in $p_v \& p_e$	Robust and accurate	10	9
1 st non-unique forbidden	0,1	-1			24	38
Main ($\varphi_{IBD} \ge 1\%$)			Nuclear struct. calcul.	Advanced calculation	6	27
Others			C opprovimation	tion Unknown accuracy	18	11
$n^{ ext{th}}$ non-unique forbidden	n	$(-1)^{n}$	ς-αρριοχιπατιοη		3	1

CLASSIFICATION OF β^- TRANSITIONS

Fluxes for typical PWR fission fractions

NON-UNIQUE FORBIDDEN SHAPE FACTOR

- No simple expression
 - ▷ Depends on **transition matrix elements** connecting nuclear states
 - \succ Nuclear structure calculations or ξ -approximation

eta-decay type	ΔJ	$\pi_i \pi_j$	Shape factor	Calculation	ν̄ _e [%]	IBD [%]
Allowed	0,1	+1	1	Debugé and accurate	61	47
Unique forbidden	n + 1	$(-1)^{n}$	Polynomial in $p_v \& p_e$	Robust and accurate	10	9
1 st non-unique forbidden	0,1	-1			24	38
Main ($\varphi_{IBD} \ge 1\%$)			Nuclear struct. calcul.	Advanced calculation	6	27
Others			C on provimation	Unknown accuracy	18	11
n^{th} non-unique forbidden	п	$(-1)^{n}$	ς-αρριοχιπατιοη		3	1

CLASSIFICATION OF β^- **TRANSITIONS**

Fluxes for typical PWR fission fractions

NON-UNIQUE FORBIDDEN SHAPE FACTOR

- No simple expression
 - Depends on transition matrix elements connecting nuclear states
 - \triangleright Nuclear structure calculations or ξ -approximation

ξ-approximation

 α : fine structure constant

• W₀: max available energy

for the transition

$$2\xi = \alpha Z/R_n \gg W_0$$

- R_n: radius of the daughter
- ▷ If verified: n^{th} non-unique ~ $(n-1)^{\text{th}}$ unique
- ▷ Applied to all non-unique transitions → induce mismodeling
 - Except 23 important non-unique transitions



NUCLEAR STRUCTURE CALCULATION (NSC)

- β -decay = single nucleon transition
- Nuclear state = superposition of nucleon states
- Non-unique shape factor calculation with NuShellX program
 - ▷ NSC very time consuming (man & cpu)
 - Comprehensive calculation for 23 important non-unique transitions
 - Uncertainty derived from comparison to allowed spectrum
 - ▷ No general nor systematic trend in non-unique shape factors

⇒ Non-unique forbidden branches treated as uncorrelated



\Rightarrow Simplistic linear model used for uncertainty of ξ -approx. non-unique transitions

NUCLEAR STRUCTURE CALCULATION (NSC)



 \Rightarrow IBD yield decreased by (1.3 \pm 0.2)% compared to full ξ -approximation

• Q_{β} energy

Fission yield (FY)

b. Nuclear data content



 \Rightarrow Summation method requires many input data

FISSION YIELD DATA

Discrepancies between cumulative FY data



- \Rightarrow Impacts fission spectrum shape
- ⇒ Impacts IBD yields 235 U ~ 0.5% 239 Pu ~ 2% 238 U ~ 3% 241 Pu ~ 2%



FISSION YIELD DATA

Covariance matrix for cumulative FY

- Correlations derived from evaluation process
 - No correlation from fission process modeling and experimental data
- No inter-actinide correlations
 - Needed for PWR

	JEFF-3.3	ENDF/B-VIII.0	JENDL-5
Source	Matthew	<u>s et al. (2021)</u>	Provided in JENDL
$\sigma_{IBD}(FY)$ no cor.	~1%	~2%	~1%
$\sigma_{IBD}(FY)$ with cor	. ~0.8%	~4%	~0.8%



 \Rightarrow Conservative choice for JEFF-3.3 is the « no correlation » case

	β ⁻ e			
		NUBASE-2020	ENSDF-2020	
	²³⁵ U	793	566	
	²³⁸ U	778	536	
	²³⁹ Pu	851	625	
	²⁴¹ Pu	860	603	
R	$\bar{\nu}_{e}$ flux co	ontribution [%]	97	
P	IBD yield	contribution [%]	92	





b. Nuclear data content

		β [−] en	
		NUBASE-2020	ENSDF-2020
	²³⁵ U	793	∖ 448
	²³⁸ U	778	∖⊾ 419
	²³⁹ Pu	851	∖ 507
	²⁴¹ Pu	860	∖ 485
R	\mathbf{v}_{e} flux contribution [%]		՝ 55
Ъ	IBD yield	d contribution [%]	⊳ 27



100

90

80



Preliminary

b. Nuclear data content

		β^- emitters from JEFF-3.3				
		NUBASE-2020	ENSDF-2020	TAGS		
	²³⁵ U	793	448	84		
	²³⁸ U	778	419	83		
	²³⁹ Pu	851	507	84		
	²⁴¹ Pu	860	485	84		
/R	$\overline{\nu}_e$ flux c	ontribution [%]	55	36		
2 2	IBD yield contribution [%]		27	55		





Quality of nuclear data



 \Rightarrow IBD yield decreased by 8% with TAGS data

			β [−] em	itters from JEI
		NUBASE-2020	ENSDF-2020	TAGS*
	²³⁵ U	793	448	84 (29)
	²³⁸ U	778	419	83 (29)
	²³⁹ Pu	851	507	84 (29)
	²⁴¹ Pu	860	485	84 (29)
/R	$\bar{\nu}_e$ flux co	ontribution [%]	55	36 (14)
Ъ	IBD yield contribution [%]		27	55 (11)

*Residual Pandemonium in parenthesis, list from INDC(NDS) - 0551. IAEA (2009) and INDC(NDS) - 0676. IAEA (2015)

Residual Pandemonium effect (RP) in ENSDF data

- RP WPEC-25
 - ▷ 29 isotopes identified by IAEA WPEC-25
 - ► IBD contribution: 10-12%

⇒ Measurements needed, meanwhile RP correction is applied



Quality of nuclear data

- Acceptable: TAGS, ENSDF
- Questionable: residual Pandemonium
 - 29 isotopes identified
 - ▷ Measurement needed

b. Nuclear data content

RESIDUAL PANDEMONIUM CORRECTION

Buiding

[%]

1.00E+01

1.00E+00

1.00E-01

1.00E-02

1.00E-03

1.00E-04

1.00E-05

- Correction + uncertainty based on 81 isotopes having both TAGS and ENSDF data ٠
- Correction = average ratio TAGS/ENSDF ٠
- Uncertainty = dispersion of ratios
 - Fully correlated between isotopes and actinides ►



b. Nuclear data content

RESIDUAL PANDEMONIUM CORRECTION

Testing on ²³⁵U

- ²³⁵U IBD yield compared to using only ENSDF
 - Using TAGS data \rightarrow -7.7%
 - Using RP correction \rightarrow (-7.2 ± 10.5)%









- Questionable: residual Pandemonium
 - 29 isotopes identified
 - ▷ Measurement needed

			β [−] em	itters from JEI
		NUBASE-2020	ENSDF-2020	TAGS*
	²³⁵ U	793	448	84 (29)
	²³⁸ U	778	419	83 (29)
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PHENOMENOLOGICAL DECAY STRENGHT MODEL

- 1 parameter Gamow-Teller strength model
- Generate missing transitions for all fission products from ENSDF
 - Correct Pandemonium effect and missing transitions
- Letourneau et al., PRL 130, 021801 (2023)
- \Rightarrow Very good agreement with STEREO





Quality of nuclear data

- Acceptable: TAGS, ENSDF
- Questionable: residual Pandemonium
 - 29 isotopes identified
 - ▷ Measurement needed

	β^- emitters from JEFF-3.3					
	NUBASE-2020	ENSDF-2020	TAGS	Direct β*		
²³⁵ U	793	448	84 (29)	44		
²³⁸ U	778	419	83 (29)	44		
²³⁹ Pu	851	507	84 (29)	44		
²⁴¹ Pu	860	485	84 (29)	44		
မှု $\bar{\nu}_e$ flux contribution [%]		55	36 (14)	8		
▲ IBD yield	d contribution [%]	27	55 (11)	13		

*Rudstam et al., At. Data Nucl. Data Tables 45(2):239-320 (1990)

Direct β measurements are Pandemonium-free

- Priority over ENSDF but after TAGS
- β spectra converted to $\bar{\nu}_e$ spectra

 \Rightarrow IBD yield decreased by (4.8 \pm 1.4)% with Direct β measurements



Quality of nuclear data

- Acceptable: TAGS, ENSDF, Direct β
- Questionable: residual Pandemonium

b. Nuclear data content

	β^- emitters from JEFF-3.3					
	NUBASE-2020	ENSDF-2020	TAGS	Direct β	No data	
²³⁵ U	793	448	84 (29)	44	217	
²³⁸ U	778	419	83 (29)	44	232	
²³⁹ Pu	851	507	84 (29)	44	216	
²⁴¹ Pu	860	485	84 (29)	44	247	
 <i>w̄</i>_e flux contribution [%] ▲ IBD yield contribution [%] 		55	36 (14)	8	1	
		27	55 (11)	13	5	

How to model nuclides with no data (NND) ?

- Different modelings already tested in other summation models
 - $rac{} Q_{\beta}$ model with n branches, Gross theory
 - ▷ No modeling uncertainty

⇒ Measurements needed, meanwhile modeling of NND + uncertainty



Quality of nuclear data

- Acceptable: TAGS, ENSDF, Direct β
- Questionable: residual Pandemonium
- Poor: nuclides with no data

Important >7 MeV

POOL MODELING OF NUCLIDES WITH NO DATA (NND)

• For each NND, spectrum + covariance matrix derived from pool of isotopes with data

Pool selection

- Isotope with data such that Q_{β} within $\pm 10\%$ of the NND Q_{β}
 - ► 10-100 isotopes with data
- Spectrum = pool average
- Covariance matrix = pool dispersion
 - Uncertainties uncorrelated between isotopes
 - Cover other NND models at isotope level





FRACTIONAL UNCERTAINTY

PWR								
$\langle \sigma_{\rm IB} \rangle$	D	6.08						
	Uncertainty	Abbrev.	Method	[%]				
	Endpoint + Spin-parity	E ₀ + Jπ	MC	0.1				
	Branching ratio + β^- intensity	$BR + I_{\beta}$	MC + Analytic	0.4				
AT A	Residual Pandemonium	RP	Analytic	2.5				
DA	Tengblad	TG	Analytic	1.5				
	Nuclides with no data	NND	Pool modeling	0.8				
	Fission yield	FY	Analytic	~0.7				
	Fission fraction		Analytic	~0.7				
	Weak magnetism	WM	Model comparison	0.3				
Ű	Radiative corrections	RC	Model comparison	0.1				
Ë	Non-unique transitions	NU	Model comparison	0.4				
Ō	Nuclear struct. calcul.	NSC		0.2				
Ĕ	 ξ-approximation 	ξ		0.3				
	IBD cross-section		Analytic	0.1				
	TOTAL			3.1				

NORMALIZATION UNCERTAINTY



⇒ Uncertainty budget dominated by RP and TG (+ NND at high energy)



IBD yields (10 ⁻⁴³ cm ² /fission)	
²³⁵ U:	6.25 ± 0.21
²³⁸ U:	10.01 ± 0.32
²³⁹ Pu:	4.48 ± 0.15
²⁴¹ Pu:	6.58 ± 0.21

 \Rightarrow IBD yield uncertainty budget \sim 3%



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3. Preliminary comparisons

a. Integral measurements

Predictions and Bugey-4 taken from Giunti et al., Phys. Lett. B, 829, 137054 (2022)

¹: <u>Phys. Rev. Lett. 123, 111801 (2019)</u>

- ²: Phys. Rev. D 104, L111301 (2021)
- ³: Phys. Rev. Lett. 125, 201801 (2020)



- 235 U, 238 U and 239 Pu : BESTIOLE consistent within $\sim 1\sigma$ with other data
- ²⁴¹Pu: small tension with other data $(1.5 2\sigma)$
 - Important contribution of NND in BESTIOLE

DB / BESTIOLE = 0.982 \pm 0.015 (exp) \pm 0.031 (model)

DB / HM = 0.945 \pm 0.014 (exp) \pm 0.024 (model)

 \Rightarrow Significance at 0.5 σ for BESTIOLE and 1.9 σ for HM $_{35}$

All plots are preliminary

b. Spectrum shape

All plots are preliminary



IMPACT OF NND MODEL



⇒ Impact of NND modeling observed >6 MeV, important >7 MeV

3. Preliminary comparisons

b. Spectrum shape

All plots are preliminary

STEREO + PROSPECT data from <u>Almazán et ak. (2022)</u> Daya Bay + PROSPECT data from <u>An et al. (2022)</u>

RATIO OF IBD SPECTRA

Gaussian fit



²³⁵U/²³⁹Pu RATIO OF IBD SPECTRA



⇒ Good agreement with experimental IBD spectra, no significant observation of deviation in 5-7 MeV



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KEY POINTS OF BESTIOLE SUMMATION PREDICTION

Modeling of non-unique forbidden transitions

- 23 non-unique forbidden branches computed with **nuclear structure calculation**
 - ▶ IBD yield decreased by (1.3 ± 0.2)%
- ξ -approximation uncertainty at fission spectrum level \sim **0.3% uncertainty**

Impact of TAGS data

- IBD yield **decreased by 8%**
- Residual Pandemonium correction, IBD yield decreased by (2.2 ± 2.4)%
 - ► Measurement needed, can also be used to validate RP correction

Modeling nuclides with no data

- Different NND modelings impact IBD yields by 1-3 %
- Important for fission spectra above 7 MeV
 - Measurement needed, priority for high-energy spectrum comparison

Comprehensive uncertainty budget

- Uncertainty budget of summation model for the first time ever
 - Impact of FY correlations to be confirmed

Final uncertainty budget ~3%

Led by RP correction

⇒ more TAGS data should be the priority

⇒ Article in preparation, coming soon with supplementary materials

Reach of a comprehensive summation model, needed for validation

