The Summation Method with the MURE code

M. Estienne[1], M. Fallot[1*], A. Algora[2, 3], J. Briz-Monago[1], V.M. Bui[1], S. Cormon[1], W. Gelletly[4], L. Giot[1], V. Guadilla[1], D. Jordan[2], L. Le Meur[1], A. Porta[1], S. Rice[4], B. Rubio[2], J. L. Taín[2], E. Valencia[2], and A.-A. Zakari-Issoufou[1]

[*] SEN group, SUBATECH (CNRS/IN2P3, Université de Nantes, IMTA),
4, rue A. Kastler, 44307 Nantes cedex 3, France fallot@subatech.in2p3.fr

WoNDRAM 2021

Outline

- Summation Method with the MURE Code
- Individual spectra computation & Nuclear Decay Data
- Individual Spectra computation & Fission Yields
- Some (old) examples of Reactor Core Simulations
- Conclusions & Outlooks

Reactor Antineutrino Spectral Knowledge

- Over the last 40 years, many computations and improvements of the spectra
- In the frame of the quest for the theta13 mixing angle:
  - ❑ **Y. Abe et al Phys. Rev. Lett. 108, 131801, (2012)**
  - ❑ **F. P. An et al., Phys. Rev. Lett. 108, 171803 (2012).**
  - ❑ **J. K. Ahn et al., Phys. Rev. Lett. 108, 191802 (2012)**

The Double Chooz experiment has devoted efforts to new computations of reactor antineutrino spectra (mandatory for the DC 1st phase !!!)

- Two methods were re-visited in 2011:
  - ❑ The **conversion of integral beta spectra of reference measured by Schreckenbach et al. in the 1980's at the ILL reactor** (thermal fission of ^{235}U, ^{239}Pu and ^{241}Pu integral beta spectra), 2 approaches in good agreement:
    - ✓ **Use of nuclear data for realistic beta branches, Z distribution of the branches, 5 fictive beta branches… instead of 30 fictive beta branches**
    - ✓ **Correction for weak magnetism and finite size effect in both approaches**

H-M model

  - ❑ The **summation method, summing all the contributions of the fission products** in a reactor core: **only nuclear data : Fission Yields + Beta Decay properties** (several predictions from B.R. Davis et al. Phys. Rev. C 19 2259 (1979), Vogel et al. to Tengblad et al. Nucl. Phys. A 503 (1989)136)

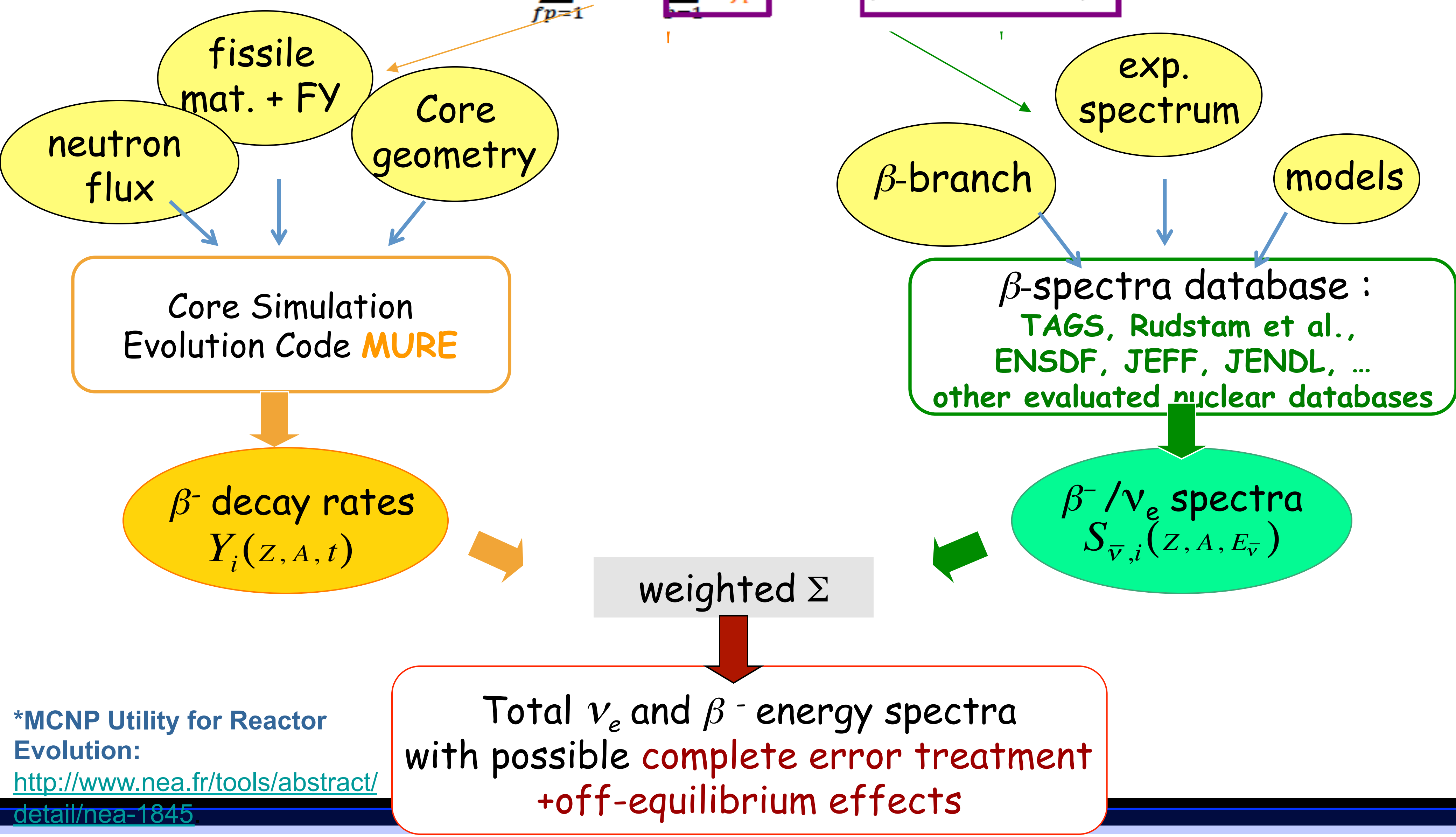
New SM model

Summation Method for Reactor Antineutrinos using the MURE Code

Summation Method

$$S_k(Z,A,E) = \sum_{fp=1}^{N_{fp}} A_{fp} \times \boxed{\sum_{b=1}^{N_b} I_{\beta\,fp}{}^{b}} \times S_{fp}{}^{b}\boxed{\left(Z_{fp}, A_{fp}, E_{0\,fp}{}^{b}, E\right))}$$

NUCLEAR DB



fissile mat. + FY

neutron flux

Core geometry

Core Simulation Evolution Code **MURE**

β^- decay rates $Y_i(Z,A,t)$

exp. spectrum

β-branch

models

β-spectra database :
TAGS, Rudstam et al., ENSDF, JEFF, JENDL, … other evaluated nuclear databases

β^-/ν_e spectra $S_{\bar{\nu},i}(Z,A,E_{\bar{\nu}})$

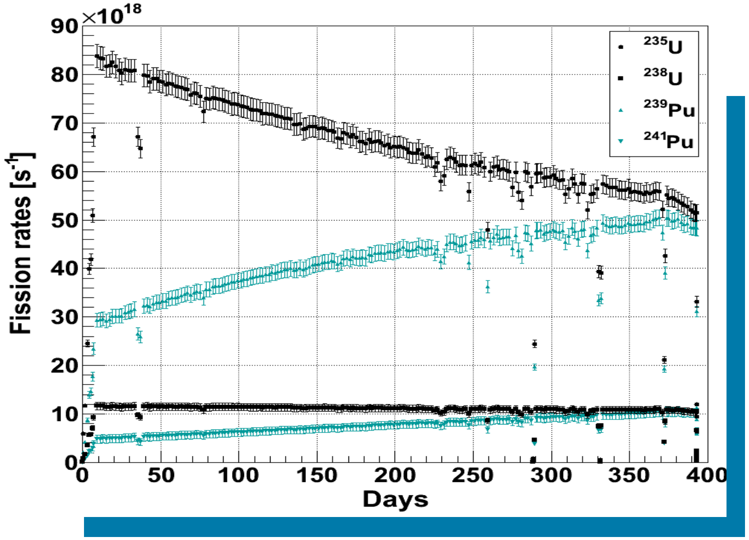
weighted Σ

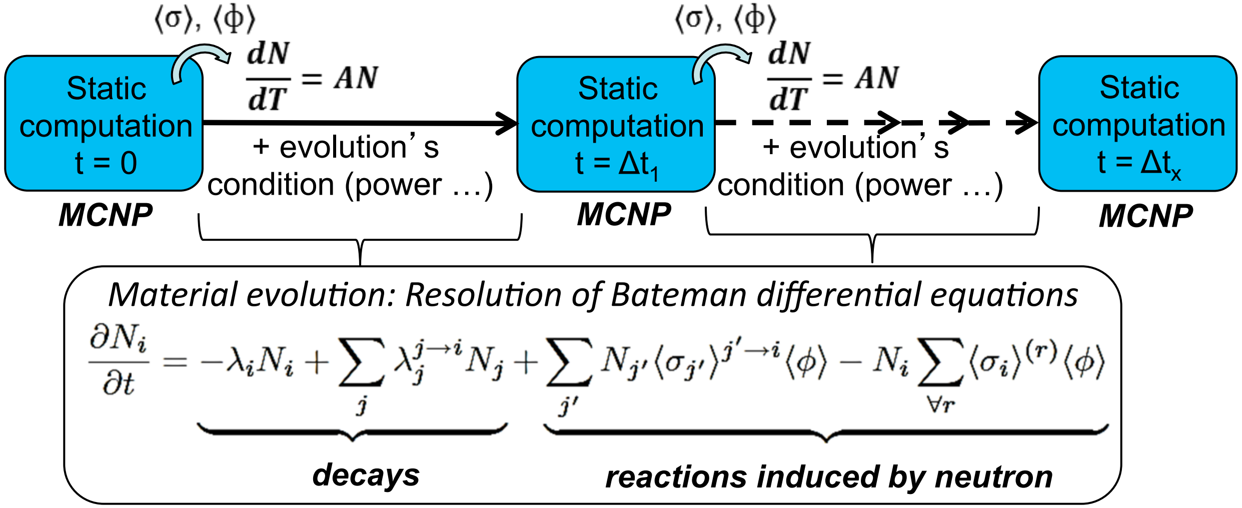
Total ν_e and β^- energy spectra with possible complete error treatment +off-equilibrium effects

***MCNP Utility for Reactor Evolution:**
http://www.nea.fr/tools/abstract/detail/nea-1845.

The MURE* Code

- **The MURE Code (MCNP Utility for Reactor Evolution) :**
  - C++ interface to the Monte Carlo code MCNP (static particle transport code)
  - Open source code available @ NEA: http://www.oecd-nea.org/tools/abstract/detail/nea-1845
  - Used for the 1st phase of the Double Chooz experiment





⟨σ⟩, ⟨ϕ⟩

Static computation t = 0

MCNP

$\frac{dN}{dT} = AN$

+ evolution’s condition (power …)

Static computation t = Δt_1

MCNP

⟨σ⟩, ⟨ϕ⟩

$\frac{dN}{dT} = AN$

+ evolution’s condition (power …)

Static computation t = Δt_x

MCNP

Material evolution: Resolution of Bateman differential equations

$$\frac{\partial N_i}{\partial t} = \underbrace{-\lambda_i N_i + \sum_j \lambda_j^{j\to i} N_j}_{\textbf{\textit{decays}}} + \underbrace{\sum_{j'} N_{j'}\langle\sigma_{j'}\rangle^{j'\to i}\langle\phi\rangle - N_i \sum_{\forall r}\langle\sigma_i\rangle^{(r)}\langle\phi\rangle}_{\textbf{\textit{reactions induced by neutron}}}$$

➡ Outputs provided: keff, neutron flux, inventory, reaction rates + adapted to compute antineutrino spectra

➡ Development of a complete core simulation with a follow up of core operating parameters

➡ Can be used also for simple geometries: individual spectra computation

A. Onillon’s PhD (Univ. Of Nantes) + Takahama benchmark: C. Jones et al. PRD 86 (2012) 012001

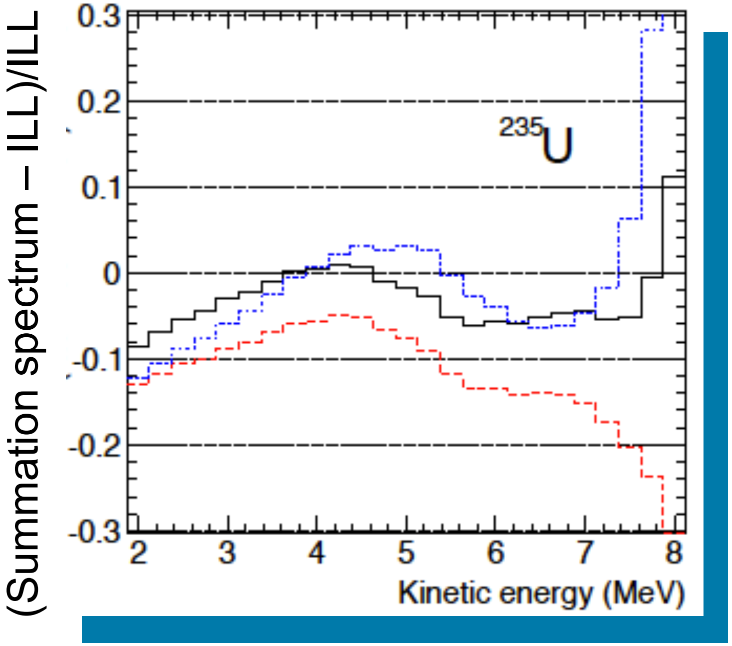
Simple Geometries: comparison to ILL-converted spectra, link with Nuclear Data

What can nuclear data bring to antineutrino spectra ?

Summation Calculations:

using Mueller and then Huber's prescriptions for spectral shape calculations, a careful selection of decay data, and fission yields from JEFF3.1:

$$N(E_\nu) = \sum_n Y_n(Z,A,t) \cdot \sum_i b_{n,i}(E_0^i) P_\nu(E_\nu, E_0^i, Z)$$



⇒ **Test of various nuclear databases: Pandemonium effect:** Overestimate of the ILL spectra @ high energy + shape distorsion

⇒ Forbiddeness is taken into account when info available except for non-unique transitions (replaced by (n-1)th unique shape)

⇒ **Requires new measurements** of FP beta decay properties

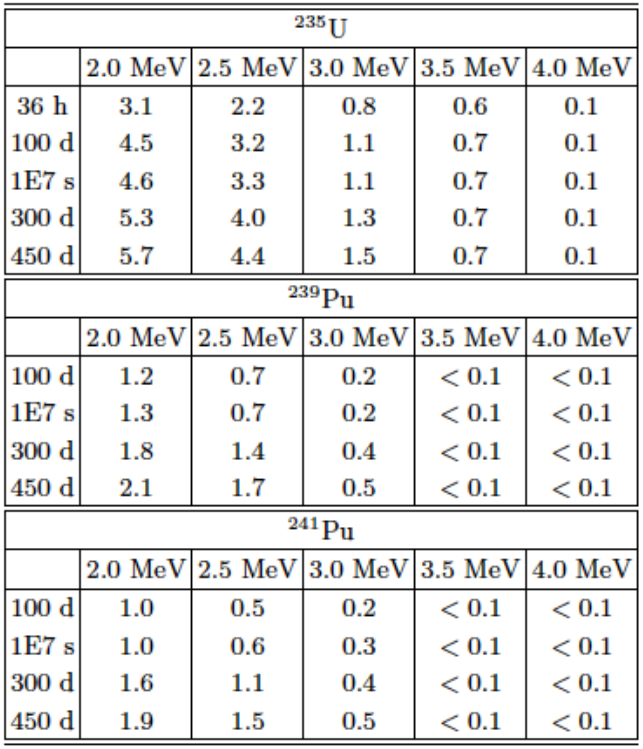
Th. Mueller et al. Phys. Rev. C 83, 054615 (2011), M. Fallot et al. Phys. Rev. Lett. 109 (2012) 202504.

The reactor antineutrino estimates suffer from the Pandemonium Effect: similar to Reactor Decay Heat (Yoshida et al. NEA/WPEC-25 (2007), Vol. 25**)**

⇒ Importance of the selection of data sets for Summation calculations: i.e. appropriate choice of decay data & fission yields

⇒ Improve systematic errors: list of nuclei to measure with TAGS experiments

Off – Equilibrium Effects



^{235}U

	2.0 MeV	2.5 MeV	3.0 MeV	3.5 MeV	4.0 MeV
36 h	3.1	2.2	0.8	0.6	0.1
100 d	4.5	3.2	1.1	0.7	0.1
1E7 s	4.6	3.3	1.1	0.7	0.1
300 d	5.3	4.0	1.3	0.7	0.1
450 d	5.7	4.4	1.5	0.7	0.1

^{239}Pu

	2.0 MeV	2.5 MeV	3.0 MeV	3.5 MeV	4.0 MeV
100 d	1.2	0.7	0.2	< 0.1	< 0.1
1E7 s	1.3	0.7	0.2	< 0.1	< 0.1
300 d	1.8	1.4	0.4	< 0.1	< 0.1
450 d	2.1	1.7	0.5	< 0.1	< 0.1

^{241}Pu

	2.0 MeV	2.5 MeV	3.0 MeV	3.5 MeV	4.0 MeV
100 d	1.0	0.5	0.2	< 0.1	< 0.1
1E7 s	1.0	0.6	0.3	< 0.1	< 0.1
300 d	1.6	1.1	0.4	< 0.1	< 0.1
450 d	1.9	1.5	0.5	< 0.1	< 0.1

TABLE VII. Relative off-equilibrium correction (in %) to be applied to the reference antineutrino spectra listed in tables IV and V, for several energy bins and several irradiation times significantly longer than the reference times (12h U for and 36h for Pu). Effect of neutron captures on fission products are included and computed using the simulation of a PWR fuel assembly with the MURE code.

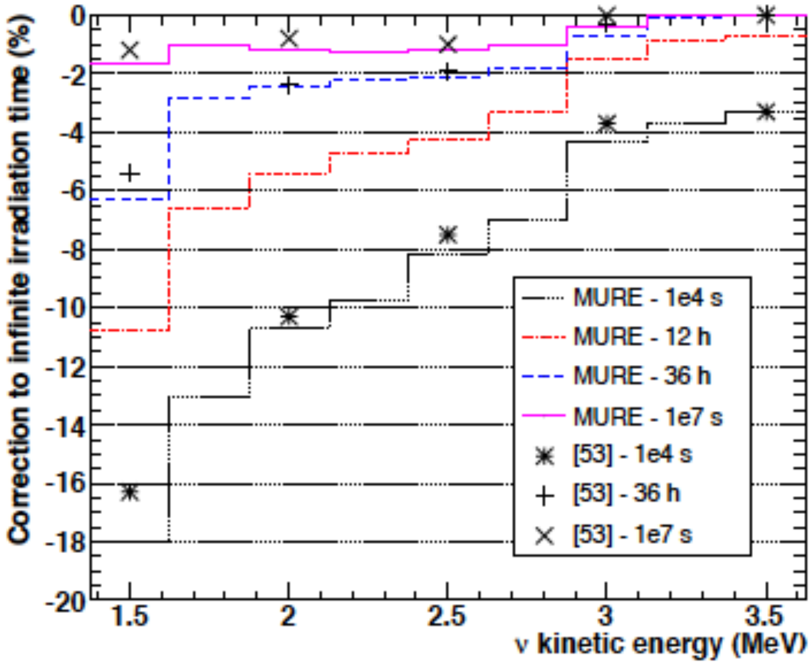


FIG. 12. Variations of the ^{235}U antineutrino spectrum for different irradiation times with respect to a reference spectrum considered at equilibrium.

Th. Mueller et al. Phys. Rev. C 83, 054615 (2011)

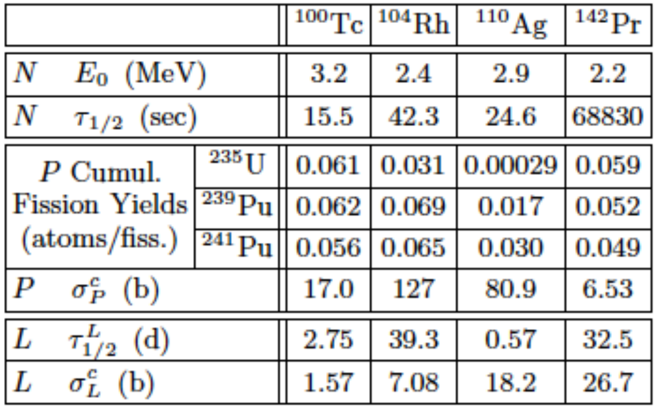
⇒ **Off-equilibrium effects on individual spectra: evolution of the fuel + neutron capture.** Have to be evaluated specifically with a realistic neutron energy distribution

⇒ **Naturally included in full core or assembly simulations with MURE**

⇒ **Accounted for about 0.5% in the reactor anomaly**

Off-Equilibrium Effects

- Studied in more details for typical PWR antineutrino spectra in:
  - ❑ V. I. Kopeikin,L.A. Mikaelyan, V. V. Sinev, arXiv:hep-ph/0110290v1
  - ❑ V. I. Kopeikin,L.A. Mikaelyan, V. V. Sinev, Phys. Atom. Nucl. 67, 11 (2004),arXiv:hep-ph/0308186v1
  - ❑ P. Huber and P. Jaffke, Phys. Rev. Lett. 116, 122503 (2016)



		^{100}Tc	^{104}Rh	^{110}Ag	^{142}Pr
N	E_0 (MeV)	3.2	2.4	2.9	2.2
N	$\tau_{1/2}$ (sec)	15.5	42.3	24.6	68830
P Cumul. Fission Yields (atoms/fiss.)	^{235}U	0.061	0.031	0.00029	0.059
	^{239}Pu	0.062	0.069	0.017	0.052
	^{241}Pu	0.056	0.065	0.030	0.049
P	σ_P^c (b)	17.0	127	80.9	6.53
L	$\tau_{1/2}^L$ (d)	2.75	39.3	0.57	32.5
L	σ_L^c (b)	1.57	7.08	18.2	26.7

TABLE I. Properties of the four selected nonlinear nuclides (N) including their beta endpoints (MeV), half-lives (sec), cumulative precursor (P) fission yields (atoms/fission), and their precursor flux-averaged thermal neutron capture cross-section (b) taking the thermal flux from Fig. 3 of Ref. [4] and the cross-sections from CINDER [5]. Also provided are the long-lived feeder parent (L) neutron capture cross-sections and half-lives.

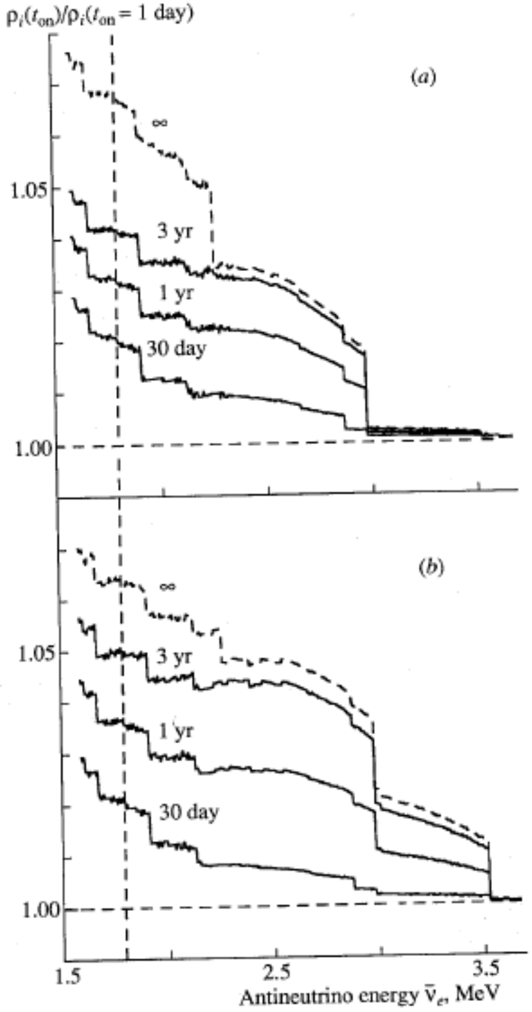


Figure 1. Ratio of the antineutrino spectra for (a) ^{235}U and (b) ^{239}Pu fission to the spectrum after one day of irradiation. The numbers on the curves indicate the irradiation time.

Anti-ν Spectra: Pandemonium Effect & TAGS

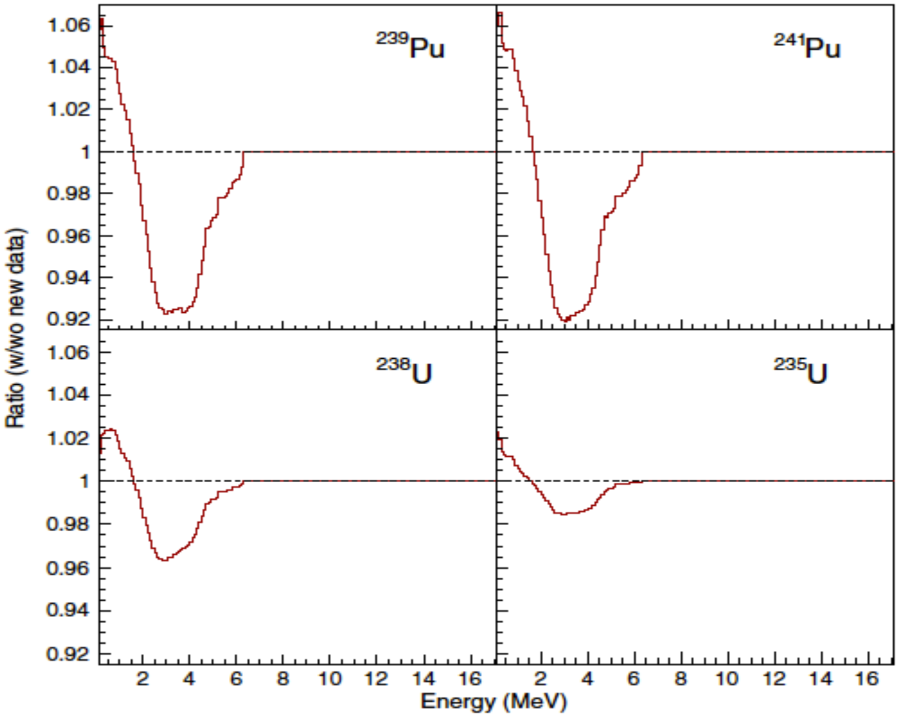
Taking into consideration the TAS data of the $^{102;104–107}$Tc, ^{105}Mo, and ^{101}Nb isotopes measured @ Jyväskylä by the Valencia team for Decay Heat

☐ ~850 nuclei included

☐ Noticeable deviation from unity (1.5 to 8% decrease)

☐ Change in the flux (presented later)

M. Fallot *et al.*, PRL 109, 202504 (2012)



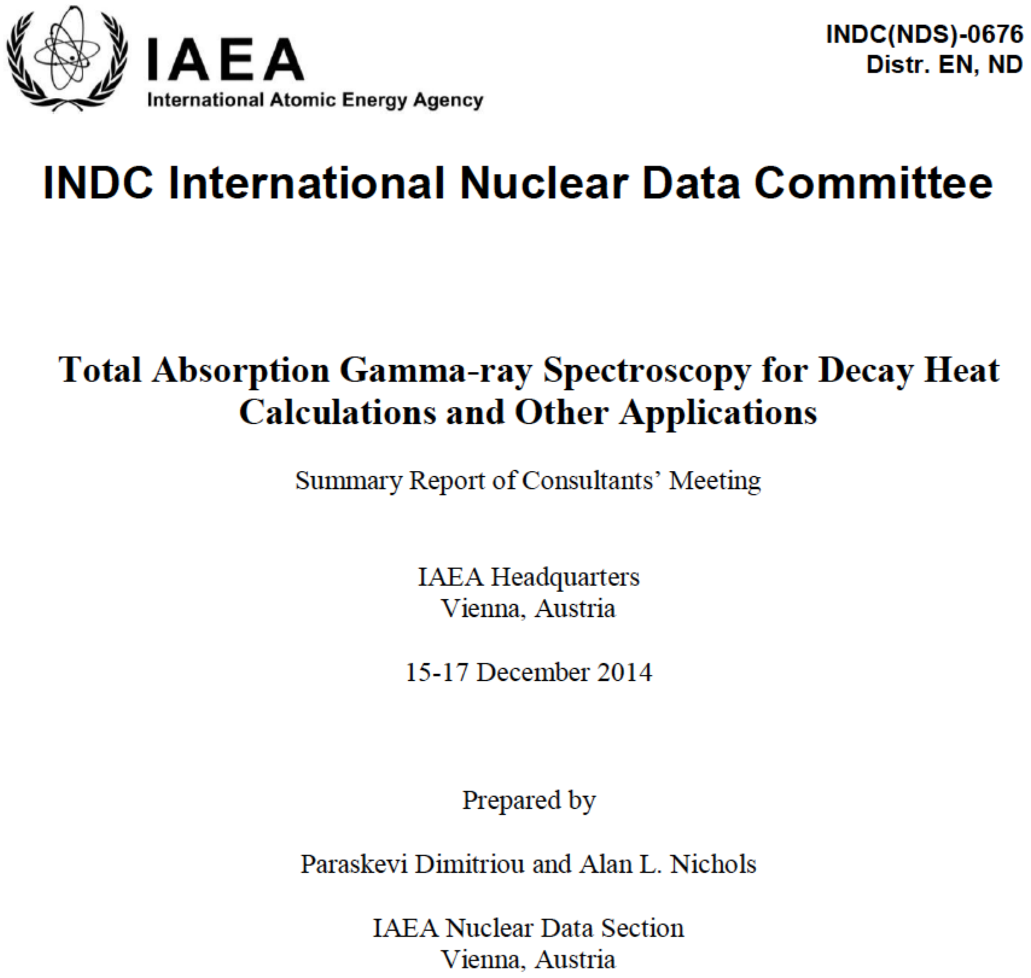
⇒ **Relative Effects of the 2012 TAS data on the Antineutrino Spectra: typical from Pandemonium effect + the inclusion of Pandemonium free data increases the spectrum below 2-3 MeV and decreases it above**

⇒ **The Nantes – Valencia collaboration started with their first TAGS measurements for antineutrino spectra in Jyväskylä as soon as 2009 !**

⇒ **Triggered the nuclear experimental efforts**

TAGS’ Consultant Meeting

Coordinated by P. Dimitriou, IAEA ND section



IAEA
International Atomic Energy Agency

INDC(NDS)-0676
Distr. EN, ND

INDC International Nuclear Data Committee

Total Absorption Gamma-ray Spectroscopy for Decay Heat Calculations and Other Applications

Summary Report of Consultants’ Meeting

IAEA Headquarters
Vienna, Austria

15-17 December 2014

Prepared by

Paraskevi Dimitriou and Alan L. Nichols

IAEA Nuclear Data Section
Vienna, Austria

TAGS' Consultant Meeting: List of contributors

Contains table of priorities for decay heat, antineutrino spectra and info about β-n emitters

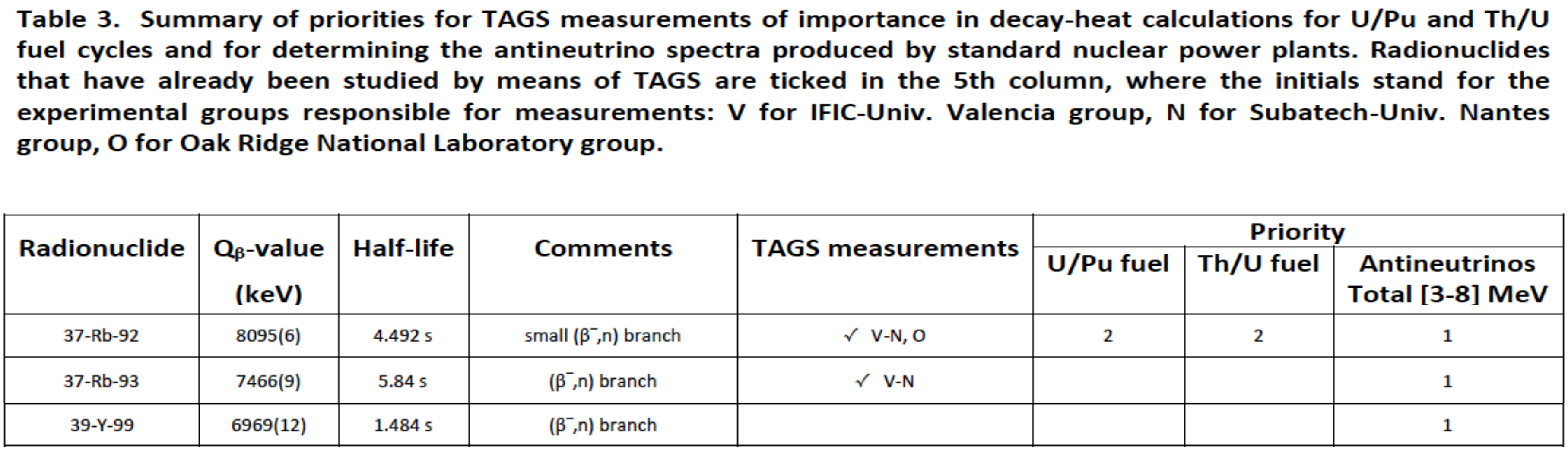


Table 3. Summary of priorities for TAGS measurements of importance in decay-heat calculations for U/Pu and Th/U fuel cycles and for determining the antineutrino spectra produced by standard nuclear power plants. Radionuclides that have already been studied by means of TAGS are ticked in the 5th column, where the initials stand for the experimental groups responsible for measurements: V for IFIC-Univ. Valencia group, N for Subatech-Univ. Nantes group, O for Oak Ridge National Laboratory group.

Radionuclide	Q_β-value (keV)	Half-life	Comments	TAGS measurements	Priority		
					U/Pu fuel	Th/U fuel	Antineutrinos Total [3-8] MeV
37-Rb-92	8095(6)	4.492 s	small (β^-,n) branch	✓ V-N, O	2	2	1
37-Rb-93	7466(9)	5.84 s	(β^-,n) branch	✓ V-N			1
39-Y-99	6969(12)	1.484 s	(β^-,n) branch				1

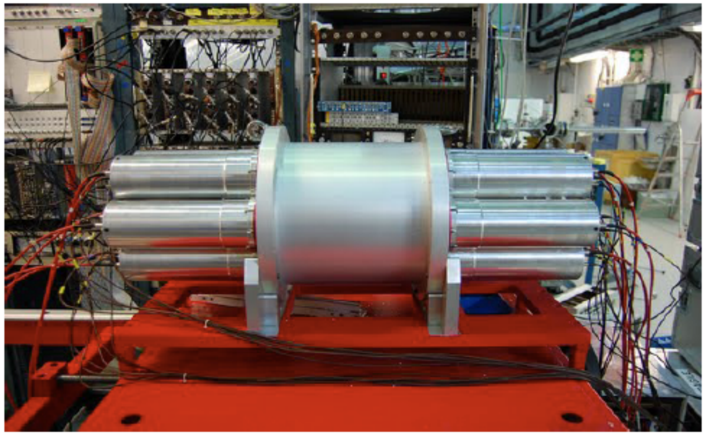
Antineutrino tables were made using the Summation Model from M. Fallot et al. PRL 2012, that was in agreement with A. Sonzogni et al. PRC 91, 011301(R) (2015)

The meetings organized by IAEA-NDS gather evaluators, experimentalists and theoreticians around a given topic. Part of the job consists in sitting together and **go through the data of each selected nucleus to critically assess the quality of the existing data.**

Nantes – Valencia Proposals: 2 TAGS Campains at IGISOL Jyväskylä in 2009 and 2014

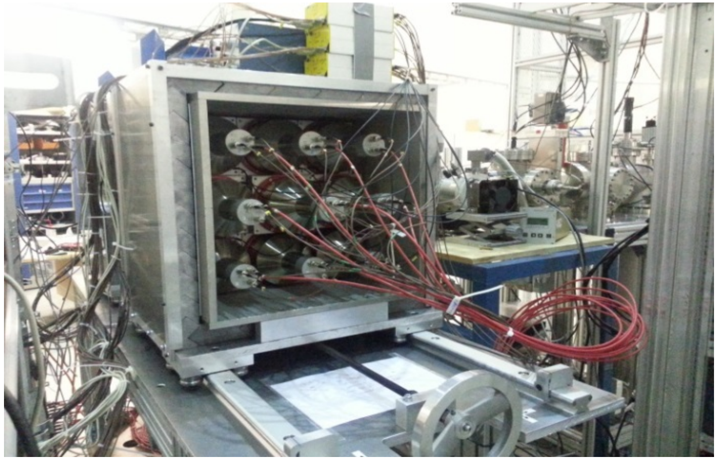
○ **2 Segmented TAGS campains @ IGISOL, Jyväskylä:**

○ ROCINANTE (IFIC Valencia/Surrey):



- ✓ **12 BaF_2 covering ~4π**
- ✓ **Detection efficiency of γ ray cascade >80% (up to 10 MeV)**
- ✓ **Coupled with a Si detector for β**
- ✓ **7 nuclei (4 delayed neutron emitters) measured (6 for DH and 2 for anti-ν)**

○ DTAS (IFIC Valencia):



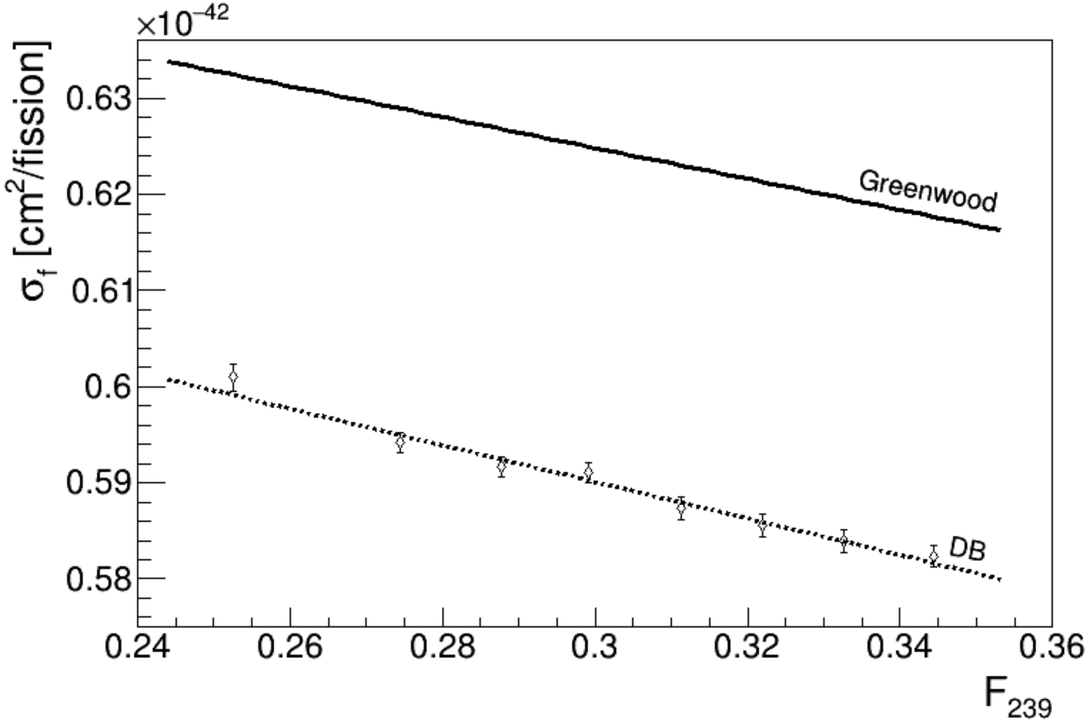
- ✓ **18 NaI(Tl) crystals of 15cm×15cm×25 cm**
- ✓ **Individual crystal resolutions: 7-8%**
- ✓ **Total efficiency: 80-90%**
- ✓ **Coupled with plastic scintillator for β**
- ✓ **12 nuclei for anti-ν measured & 11 for DH**

J.L. Tain et al., NIM A 803 (2015) 36
V. Guadilla et al., NIM A (2018) 910 (2018) 79-89

Impact of TAGS measurements over the decade

- The IBD yields dependency with F239 including TAGS data published in 2012, 2015, 2017 and 2019 has been calculated using our summation calculation

M. Fallot et al. PRL 109,202504 (2012), **SM-2012**
A.A. Zakari-Issoufou et al. PRL 115, 102503 (2015), **SM-2015**
E. Valencia et al., PRC 95, 024320 (2017) + S. Rice et al. PRC 96 (2017) 014320 **SM-2017**
V. Guadilla et al. PRL122, (2019) 042502 **SM-2018**



- Impact of the inclusion of the TAGS data (Pandemonium free):

⇒ **Systematic reduction of the detected flux**

⇒ **Systematic reduction of the discrepancy with Daya Bay results**

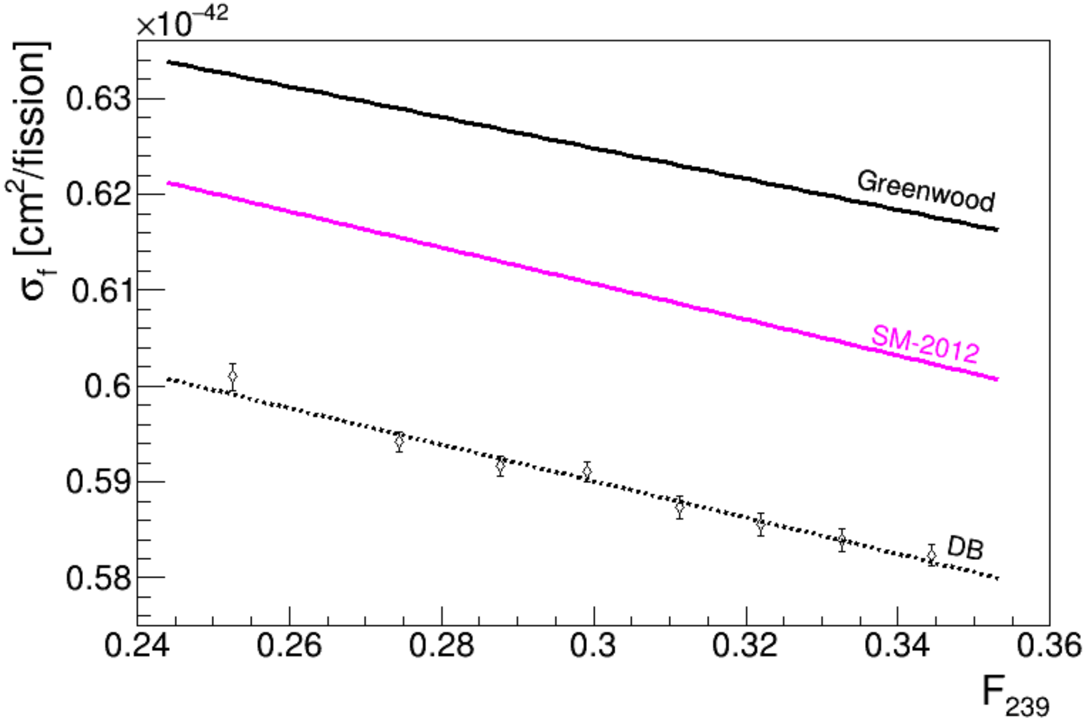
⇒ Implies an increasingly smaller discrepancy with the inclusion of future TAGS data, **leaving less and less room for a reactor anomaly**.

M. Estienne et al. PRL 123, (2019) 022502 http://arxiv.org/abs/1904.09358

Impact of TAGS measurements over the decade

- The IBD yields dependency with F239 including TAGS data published in 2012, 2015, 2017 and 2019 has been calculated using our summation calculation

M. Fallot et al. PRL 109,202504 (2012), **SM-2012**
A.A. Zakari-Issoufou et al. PRL 115, 102503 (2015), **SM-2015**
E. Valencia et al., PRC 95, 024320 (2017) + S. Rice et al. PRC 96 (2017) 014320 **SM-2017**
V. Guadilla et al. PRL122, (2019) 042502 **SM-2018**



- Impact of the inclusion of the TAGS data (Pandemonium free):

⇒ **Systematic reduction of the detected flux**

⇒ **Systematic reduction of the discrepancy with Daya Bay results**

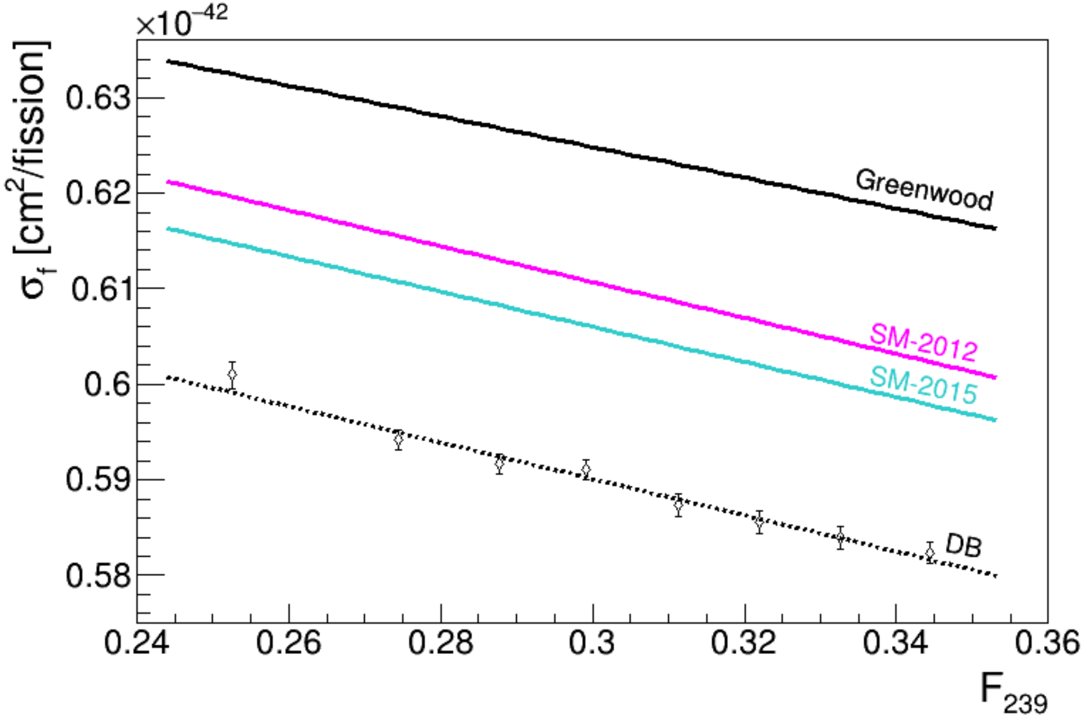
⇒ Implies an increasingly smaller discrepancy with the inclusion of future TAGS data, **leaving less and less room for a reactor anomaly**.

M. Estienne et al. **PRL 123, (2019) 022502** http://arxiv.org/abs/1904.09358

Impact of TAGS measurements over the decade

- The IBD yields dependency with F239 including TAGS data published in 2012, 2015, 2017 and 2019 has been calculated using our summation calculation

M. Fallot et al. PRL 109,202504 (2012), **SM-2012**
A.A. Zakari-Issoufou et al. PRL 115, 102503 (2015), **SM-2015**
E. Valencia et al., PRC 95, 024320 (2017) + S. Rice et al. PRC 96 (2017) 014320 **SM-2017**
V. Guadilla et al. PRL122, (2019) 042502 **SM-2018**



- Impact of the inclusion of the TAGS data (Pandemonium free):

⇒ **Systematic reduction of the detected flux**

⇒ **Systematic reduction of the discrepancy with Daya Bay results**

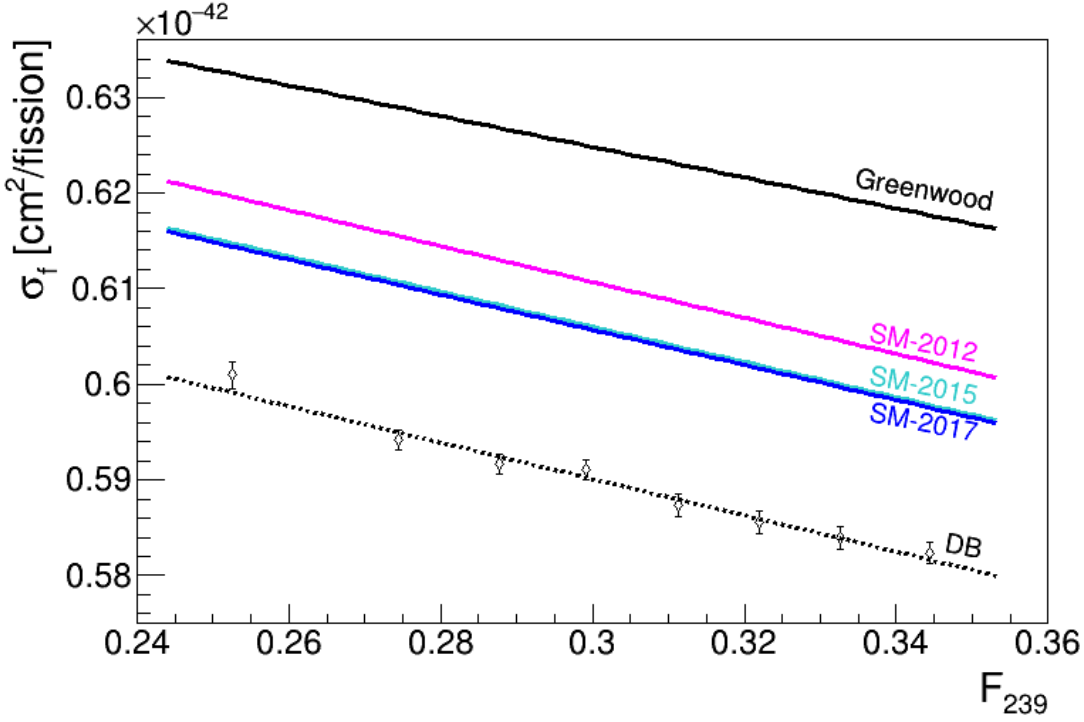
⇒ Implies an increasingly smaller discrepancy with the inclusion of future TAGS data, **leaving less and less room for a reactor anomaly**.

M. Estienne et al. PRL 123, (2019) 022502 http://arxiv.org/abs/1904.09358

Impact of TAGS measurements over the decade

- The IBD yields dependency with F239 including TAGS data published in 2012, 2015, 2017 and 2019 has been calculated using our summation calculation

M. Fallot et al. PRL 109,202504 (2012), **SM-2012**
A.A. Zakari-Issoufou et al. PRL 115, 102503 (2015), **SM-2015**
E. Valencia et al., PRC 95, 024320 (2017) + S. Rice et al. PRC 96 (2017) 014320 **SM-2017**
V. Guadilla et al. PRL122, (2019) 042502 **SM-2018**



- Impact of the inclusion of the TAGS data (Pandemonium free):

⇒ **Systematic reduction of the detected flux**

⇒ **Systematic reduction of the discrepancy with Daya Bay results**

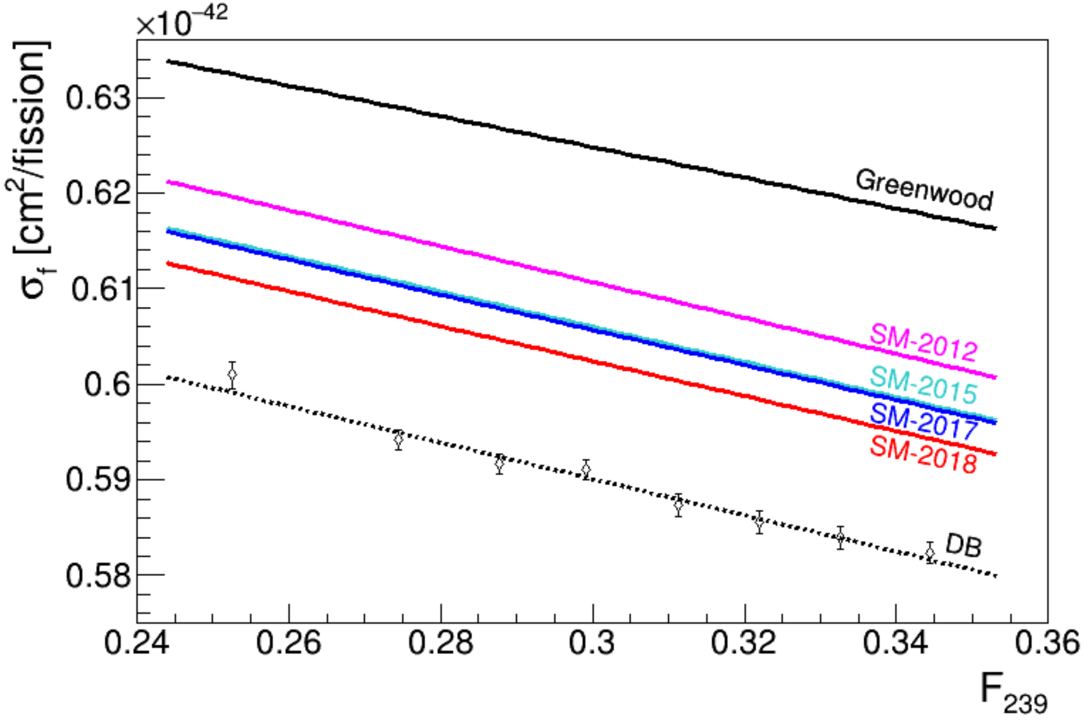
⇒ Implies an increasingly smaller discrepancy with the inclusion of future TAGS data, **leaving less and less room for a reactor anomaly**.

M. Estienne et al. **PRL 123, (2019) 022502** http://arxiv.org/abs/1904.09358

Impact of TAGS measurements over the decade

- The IBD yields dependency with F239 including TAGS data published in 2012, 2015, 2017 and 2019 has been calculated using our summation calculation

M. Fallot et al. PRL 109,202504 (2012), **SM-2012**
A.A. Zakari-Issoufou et al. PRL 115, 102503 (2015), **SM-2015**
E. Valencia et al., PRC 95, 024320 (2017) + S. Rice et al. PRC 96 (2017) 014320 **SM-2017**
V. Guadilla et al. PRL122, (2019) 042502 **SM-2018**



- Impact of the inclusion of the TAGS data (Pandemonium free):

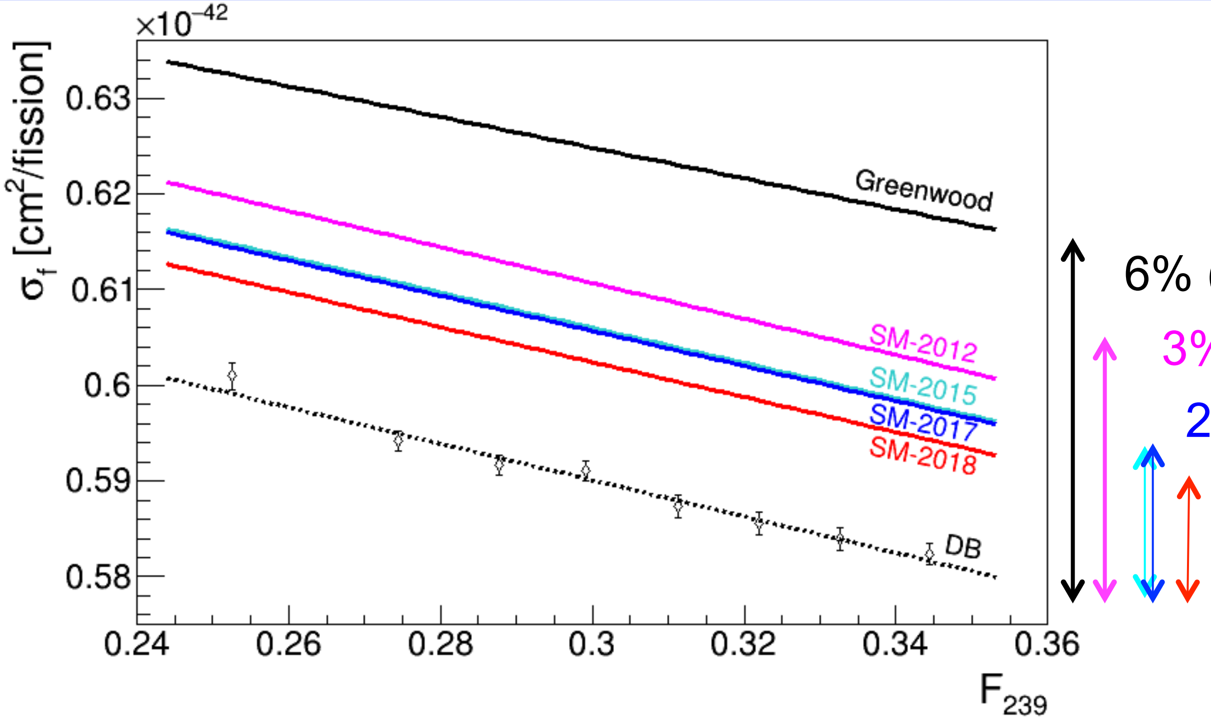
⇒ **Systematic reduction of the detected flux**

⇒ **Systematic reduction of the discrepancy with Daya Bay results**

⇒ Implies an increasingly smaller discrepancy with the inclusion of future TAGS data, **leaving less and less room for a reactor anomaly**.

M. Estienne et al. PRL 123, (2019) 022502 http://arxiv.org/abs/1904.09358

Impact of TAGS measurements over the decade



6% (Greenwood TAGS, ~Huber-Mueller)

3% (+TAGS 2012, ~< Hayes et al. 3.5%)

2.4% (+TAGS 2015 & 2017)

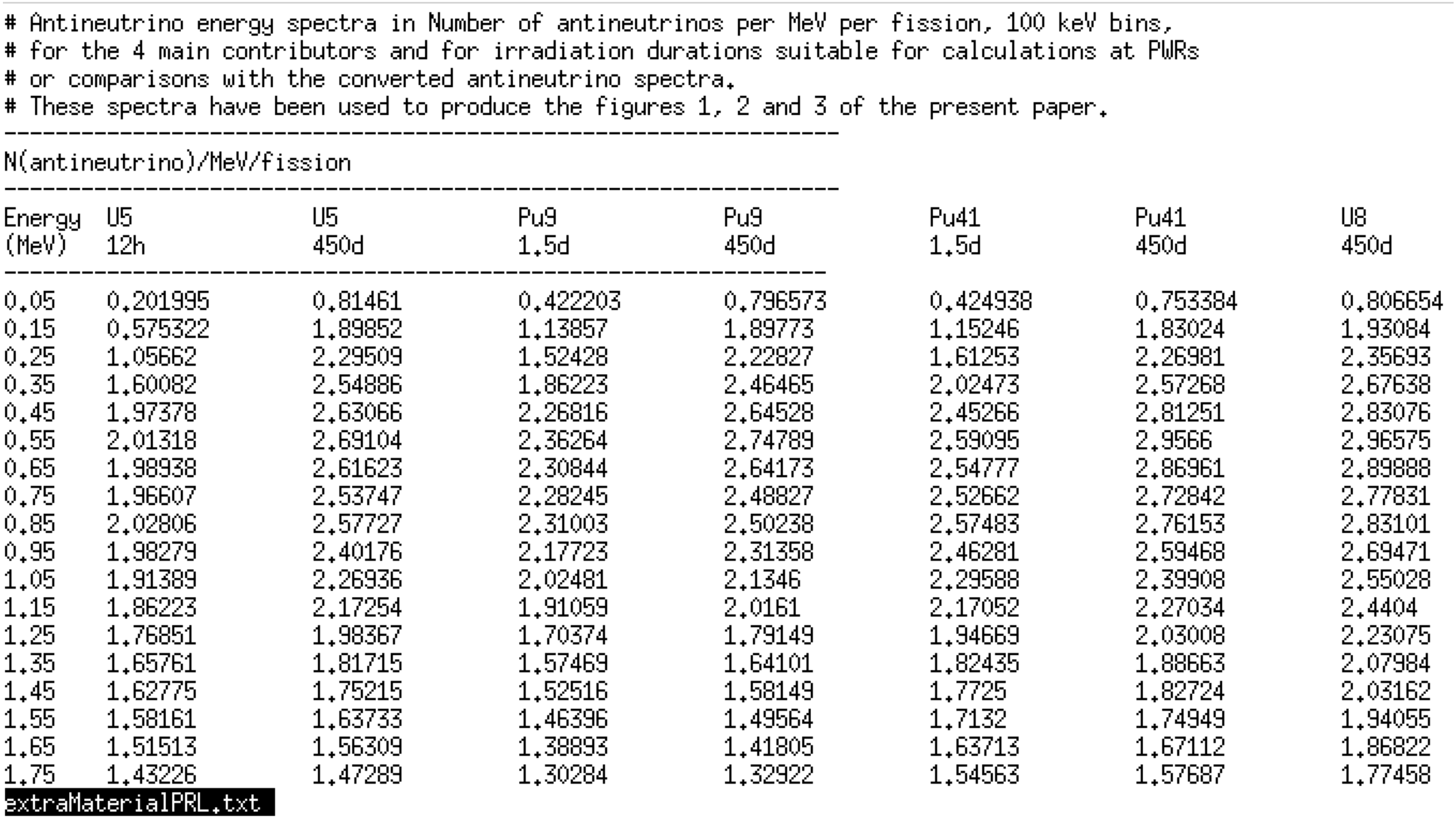
1.9% (+ TAGS 2018)

- The remaining discrepancy with the Daya Bay flux **reduces to only 1.9%**
- Even with the inclusion of the 2018 TAGS data, the **bump is still there** i.e. for the moment, it still **cannot be explained** by ingredients of the nuclear databases.
- **With the SM model, no huge discrepancy in the flux w.r.t. DB for one specific fissioning nucleus: 2.5-3% for ^{235}U and ^{239}Pu (contrary to H.-M.)** and about 1% for ^{238}U and ^{241}Pu

M. Estienne et al. **PRL 123, (2019) 022502** http://arxiv.org/abs/1904.09358

Off-Equilibrium Effects

- With M. Estienne et al. **PRL 123, (2019) 022502, was provided a supplemental material with the coordinates of the summation spectra used in the paper at 2 evolution times:**



```
# Antineutrino energy spectra in Number of antineutrinos per MeV per fission, 100 keV bins,
# for the 4 main contributors and for irradiation durations suitable for calculations at PWRs
# or comparisons with the converted antineutrino spectra.
# These spectra have been used to produce the figures 1, 2 and 3 of the present paper.
-----------------------------------------------------------------
N(antineutrino)/MeV/fission
-----------------------------------------------------------------
Energy  U5              U5              Pu9             Pu9             Pu41            Pu41            U8
(MeV)   12h             450d            1.5d            450d            1.5d            450d            450d
----------------------------------------------------------------
0.05    0.201995        0.81461         0.422203        0.796573        0.424938        0.753384        0.806654
0.15    0.575322        1.89852         1.13857         1.89773         1.15246         1.83024         1.93084
0.25    1.05662         2.29509         1.52428         2.22827         1.61253         2.26981         2.35693
0.35    1.60082         2.54886         1.86223         2.46465         2.02473         2.57268         2.67638
0.45    1.97378         2.63066         2.26816         2.64528         2.45266         2.81251         2.83076
0.55    2.01318         2.69104         2.36264         2.74789         2.59095         2.9566          2.96575
0.65    1.98938         2.61623         2.30844         2.64173         2.54777         2.86961         2.89888
0.75    1.96607         2.53747         2.28245         2.48827         2.52662         2.72842         2.77831
0.85    2.02806         2.57727         2.31003         2.50238         2.57483         2.76153         2.83101
0.95    1.98279         2.40176         2.17723         2.31358         2.46281         2.59468         2.69471
1.05    1.91389         2.26936         2.02481         2.1346          2.29588         2.39908         2.55028
1.15    1.86223         2.17254         1.91059         2.0161          2.17052         2.27034         2.4404
1.25    1.76851         1.98367         1.70374         1.79149         1.94669         2.03008         2.23075
1.35    1.65761         1.81715         1.57469         1.64101         1.82435         1.88663         2.07984
1.45    1.62775         1.75215         1.52516         1.58149         1.7725          1.82724         2.03162
1.55    1.58161         1.63733         1.46396         1.49564         1.7132          1.74949         1.94055
1.65    1.51513         1.56309         1.38893         1.41805         1.63713         1.67112         1.86822
1.75    1.43226         1.47289         1.30284         1.32922         1.54563         1.57687         1.77458
extraMaterialPRL.txt
```

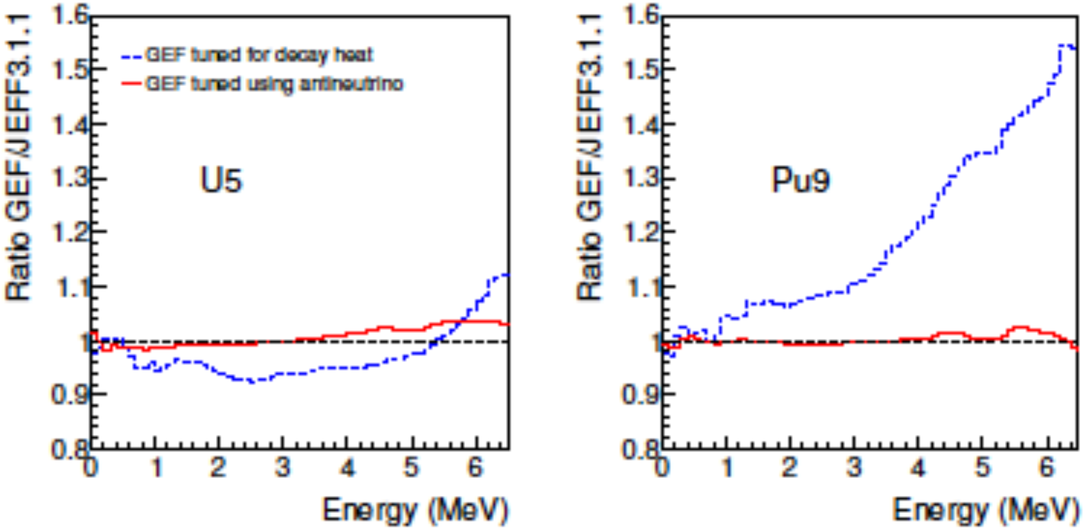
Simple Geometries: Uncertainties & Fission Yields…

Fission Yields & Antineutrinos

- The **SM spectra need uncertainties**: not trivial ! Because:
  - ☐ **Decay data:** Pandemonium effect needs to be eliminated, otherwise the quoted uncertainties in the databases have no meaning;
  - ☐ **Fission Yields**: need covariance matrices ;
- Collaboration with Karl-Heinz Schmidt in Subatech-Nantes in order to use the GEF code to study antineutrino spectra with the propagation of uncertainties:

The GEF code prediction capability for the fission yields was not good enough for antineutrino spectra:

For the first **time a careful analysis and a systematic comparison of data from different sources and evaluations with GEF have been performed to sort out the more reliable and the less trustworthy values** ;



⇒Reactor Antineutrino spectra combined with the GEF model provide a useful tool to assist fission yield data evaluation

Fission Yields & Antineutrinos

- **Estienne et al. collaborate with K.-H. Schmidt** (author of GEF with B. Jurado) for several years with the purpose to use the GEF FY with their uncertainties. First results are:
    - ➢ **a new version of the GEF code improved thanks to the antineutrino spectral studies**
    - ➢ **an assessment of the experimentally available fission yields with the GEF model showing that the discrepancies btw FY from JEFF3.1.1 and JEFF3.3 are not always understood**
    - ➢ **The ^{238}U spectrum is obtained using a realistic PWR neutron flux in GEF (improves agreement with JEFF FY)**
    - ➢ New predictions compared with the DB flux
    - ➢ New predictions of actinide antineutrino spectra for applications

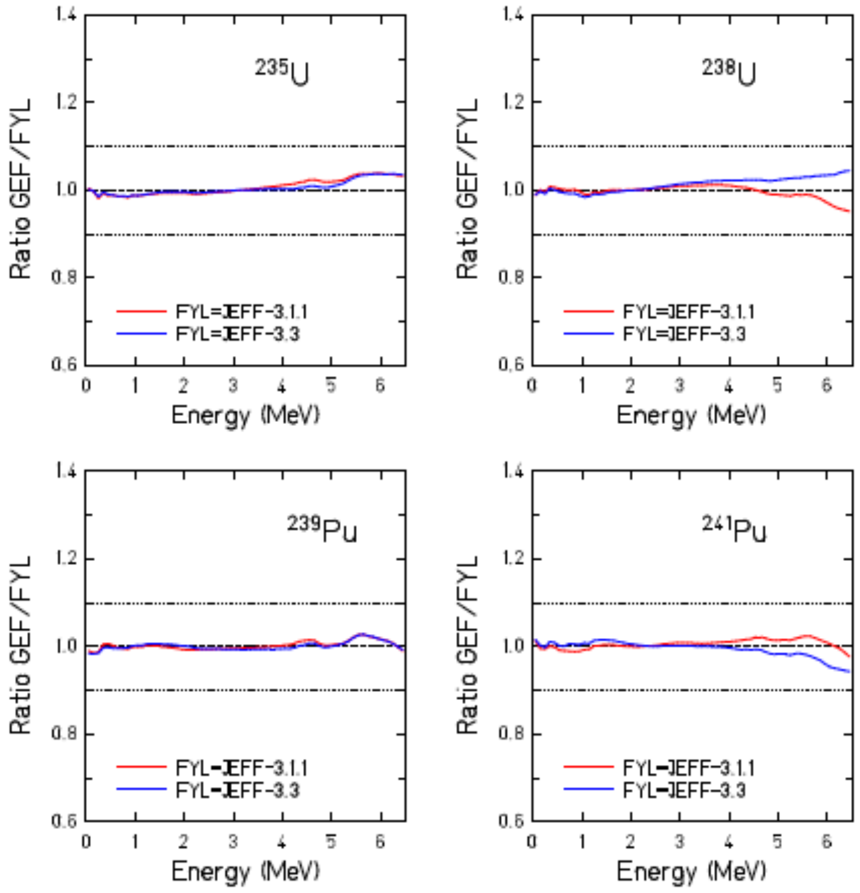
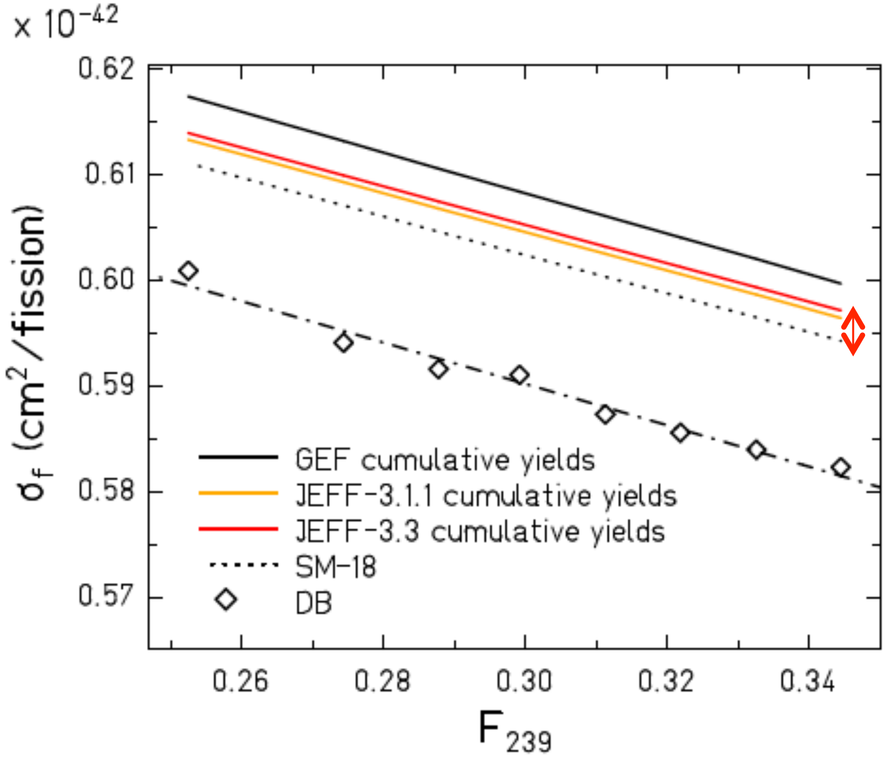


FIG. 63. Ratio of the antineutrino spectra calculated with yields from GEF and from the fission-yield libraries (FYL) JEFF-3.1.1, respectively JEFF-3.3, after tuning.

Extensive study of the quality of fission yields from experiment, evaluation and GEF for antineutrino studies and applications, K.-H.Schmidt, M.Estienne, M.Fallot, et al., Nuclear Data Sheets Volume 173, (2021), Pages 54-117, https://doi.org/10.1016/j.nds.2021.04.004

Fission Yields & Antineutrinos

- **Estienne et al. collaborate with K.-H. Schmidt** (author of GEF with B. Jurado) for several years with the purpose to use the GEF FY with their uncertainties. First results are:
  - a new version of the GEF code improved thanks to the antineutrino spectral studies
  - an assessment of the experimentally available fission yields with the GEF model showing that the discrepancies btw FY from JEFF3.1.1 and JEFF3.3 are not always understood
  - The ^{238}U spectrum is obtained using a realistic PWR neutron flux in GEF (improves agreement with JEFF FY)
  - **New predictions compared with the DB flux**
  - New predictions of actinide antineutrino spectra for applications

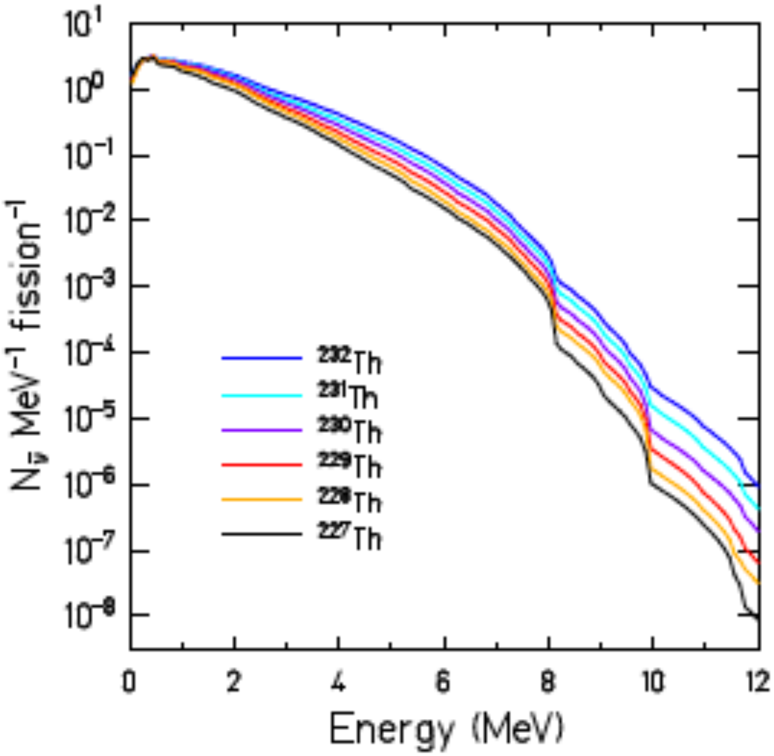


↕ : impact of off-equilibrium effects w.r.t cumulative FY: 0.5%

Extensive study of the quality of fission yields from experiment, evaluation and GEF for antineutrino studies and applications, K.-H.Schmidt, M.Estienne, M.Fallot, et al., Nuclear Data Sheets Volume 173, (2021), Pages 54-117, https://doi.org/10.1016/j.nds.2021.04.004

Fission Yields & Antineutrinos

- **Estienne et al. collaborate with K.-H. Schmidt** (author of GEF with B. Jurado) for several years with the purpose to use the GEF FY with their uncertainties. First results are:
  - ➢ **a new version of the GEF code improved thanks to the antineutrino spectral studies**
  - ➢ an assessment of the experimentally available fission yields with the GEF model showing that the discrepancies btw FY from JEFF3.1.1 and JEFF3.3 are not always understood
  - ➢ The ^{238}U spectrum is obtained using a realistic PWR neutron flux in GEF (improves agreement with JEFF FY)
  - ➢ New predictions compared with the DB flux
  - ➢ **New predictions of actinide antineutrino spectra for applications**



Extensive study of the quality of fission yields from experiment, evaluation and GEF for antineutrino studies and applications, K.-H.Schmidt, M.Estienne, M.Fallot, et al., Nuclear Data Sheets Volume 173, (2021), Pages 54-117, https://doi.org/10.1016/j.nds.2021.04.004

Reactor Monitoring, Innovative fuels…

Scenarios and reactors of interest?

- PWRs
- BWR, FBR, CANDU reactors
- Research reactor / isotope production reactors Pth >10MWth: OSIRIS, BR2
- Future reactors (PBMRs, Gen IV reactors, ADS, especially reactors using carbide, nitride, metal or molten salt fuels, advanced CANDUs…)
- MOX Management, Innovative fuels

UOx, MOX, ThUOx, PuOx, thermal neutron spectrum

^{238}U/^{239}Pu or ^{232}Th/^{233}U cycles, fast neutron spectrum

Minor Actinides, Protected Plutonium Production fuel…

Some examples of performed studies…

Short description of the Chooz Core

- **2 PWRs –N4 type (EDF electricity company), 4.25GWth each**
- **Summary of the core geometry in a few figures :**
  - 205 assemblies, each composed of 264 fuel rods
  - 4 assembly types with different :
    - geometrical characteristics
    - initial fuel composition & enrichments
  - ~ 1/3 of the assemblies with fresh fuel
  - ~ 100 assemblies with gadolinium & 100 without

x x x → **Burnup at the start of the cycle**

$$Burnup = \sum_i \langle P_{therm} \rangle_i \times time_i / Mass_{initial}$$

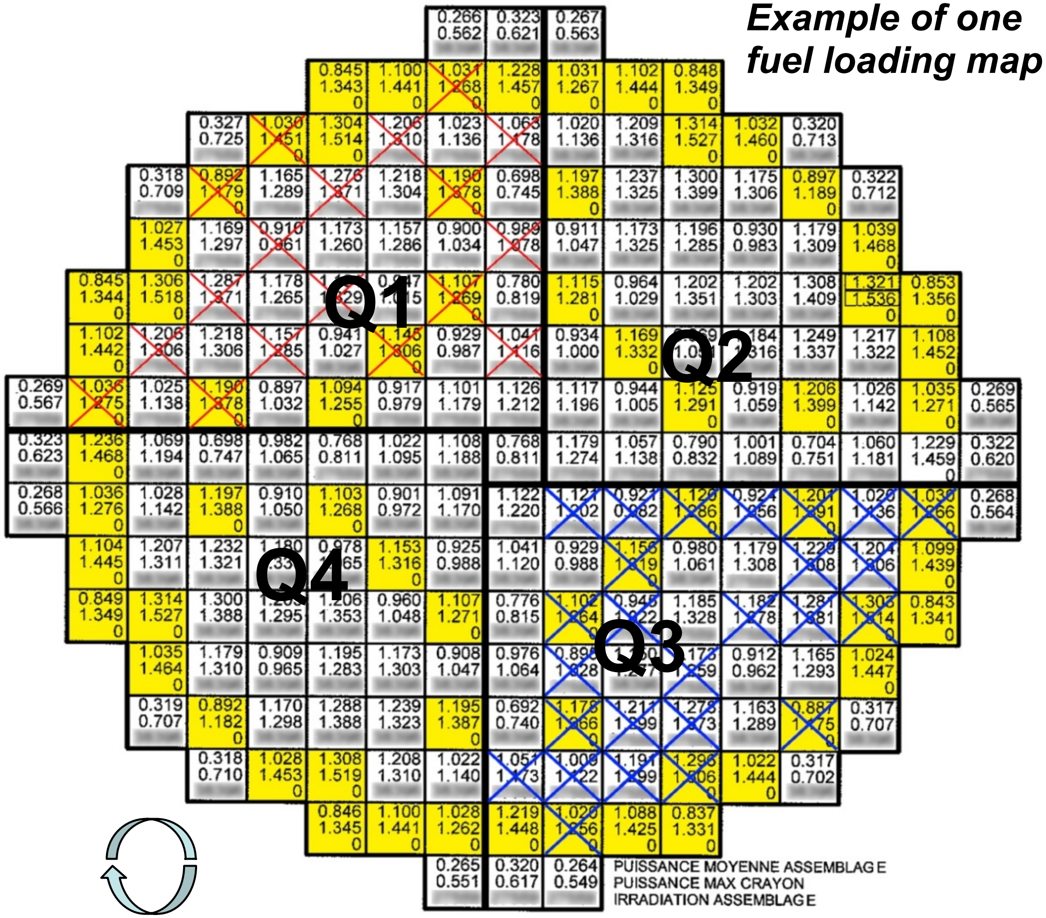
🟨 : Fresh fuel

☒ : Control rod position (first quadrant)

☒ : Gadolinum assemblies (third quadrant)

⇨ *High neutron absorber*

Example of one fuel loading map



							0.266 0.562 [redacted]	0.323 0.621 [redacted]	0.267 0.563 [redacted]							
					0.845 1.343 0	1.100 1.441 0	1.031 1.268 0	1.228 1.457 0	1.031 1.267 0	1.102 1.444 0	0.848 1.349 0					
			0.327 0.725 [redacted]	1.030 1.451 0	1.304 1.514 0	1.206 1.310 [redacted]	1.023 1.136 [redacted]	1.063 1.178 [redacted]	1.020 1.136 [redacted]	1.209 1.316 [redacted]	1.314 1.527 0	1.032 1.460 0	0.320 0.713 [redacted]			
		0.318 0.709 [redacted]	0.892 1.179 0	1.165 1.289 [redacted]	1.276 1.371 [redacted]	1.218 1.304 [redacted]	1.190 1.378 0	0.698 0.745 [redacted]	1.197 1.388 0	1.237 1.325 [redacted]	1.300 1.399 [redacted]	1.175 1.306 [redacted]	0.897 1.189 0	0.322 0.712 [redacted]		
		1.027 1.453 0	1.169 1.297 [redacted]	0.910 0.961 [redacted]	1.173 1.260 [redacted]	1.157 1.286 [redacted]	0.900 1.034 [redacted]	0.989 1.078 [redacted]	0.911 1.047 [redacted]	1.173 1.325 [redacted]	1.196 1.285 [redacted]	0.930 0.983 [redacted]	1.179 1.309 [redacted]	1.039 1.468 0		
	0.845 1.344 0	1.306 1.518 0	1.287 1.371 [redacted]	1.178 1.265 [redacted]	[illegible] 1.329 [redacted]	0.947 1.015 [redacted]	1.107 1.269 0	0.780 0.819 [redacted]	1.115 1.281 0	0.964 1.029 [redacted]	1.202 1.351 [redacted]	1.202 1.303 [redacted]	1.308 1.409 [redacted]	1.321 1.536 0	0.853 1.356 0	
	1.102 1.442 0	1.206 1.306 [redacted]	1.218 1.306 [redacted]	1.157 1.285 [redacted]	0.941 1.027 [redacted]	1.145 1.306 0	0.929 0.987 [redacted]	1.041 1.116 [redacted]	0.934 1.000 [redacted]	1.169 1.332 0	[illegible] [illegible] [redacted]	1.184 1.316 [redacted]	1.249 1.337 [redacted]	1.217 1.322 [redacted]	1.108 1.452 0	
0.269 0.567 [redacted]	1.036 1.275 0	1.025 1.138 [redacted]	1.190 1.378 0	0.897 1.032 [redacted]	1.094 1.255 0	0.917 0.979 [redacted]	1.101 1.179 [redacted]	1.126 1.212 [redacted]	1.117 1.196 [redacted]	0.944 1.005 [redacted]	1.125 1.291 0	0.919 1.059 [redacted]	1.206 1.399 0	1.026 1.142 [redacted]	1.035 1.271 0	0.269 0.565 [redacted]
0.323 0.623 [redacted]	1.236 1.468 0	1.069 1.194 [redacted]	0.698 0.747 [redacted]	0.982 1.065 [redacted]	0.768 0.811 [redacted]	1.022 1.095 [redacted]	1.108 1.188 [redacted]	0.768 0.811 [redacted]	1.179 1.274 [redacted]	1.057 1.138 [redacted]	0.790 0.832 [redacted]	1.001 1.089 [redacted]	0.704 0.751 [redacted]	1.060 1.181 [redacted]	1.229 1.459 0	0.322 0.620 [redacted]
0.268 0.566 [redacted]	1.036 1.276 0	1.028 1.142 [redacted]	1.197 1.388 0	0.910 1.050 [redacted]	1.103 1.268 0	0.901 0.972 [redacted]	1.091 1.170 [redacted]	1.122 1.220 [redacted]	1.121 1.202 [redacted]	0.921 0.982 [redacted]	1.126 1.286 0	0.924 1.256 [redacted]	1.201 1.391 0	1.020 1.136 [redacted]	1.030 1.266 0	0.268 0.564 [redacted]
	1.104 1.445 0	1.207 1.311 [redacted]	1.232 1.321 [redacted]	1.180 [illegible] [redacted]	0.978 [illegible] [redacted]	1.153 1.316 0	0.925 0.988 [redacted]	1.041 1.120 [redacted]	0.929 0.988 [redacted]	1.156 1.319 0	0.980 1.061 [redacted]	1.179 1.308 [redacted]	1.229 1.308 [redacted]	1.204 1.306 [redacted]	1.099 1.439 0	
	0.849 1.349 0	1.314 1.527 0	1.300 1.388 [redacted]	[illegible] 1.295 [redacted]	1.206 1.353 [redacted]	0.960 1.048 [redacted]	1.107 1.271 0	0.776 0.815 [redacted]	1.102 1.264 0	0.945 1.322 [redacted]	1.185 1.328 [redacted]	1.182 1.278 [redacted]	1.281 1.381 [redacted]	1.306 1.514 0	0.843 1.341 0	
		1.035 1.464 0	1.179 1.310 [redacted]	0.909 0.965 [redacted]	1.195 1.283 [redacted]	1.173 1.303 [redacted]	0.908 1.047 [redacted]	0.976 1.064 [redacted]	0.895 1.028 [redacted]	[illegible] [illegible] [redacted]	1.173 1.259 [redacted]	0.912 0.962 [redacted]	1.165 1.293 [redacted]	1.024 1.447 0		
		0.319 0.707 [redacted]	0.892 1.182 0	1.170 1.298 [redacted]	1.288 1.388 [redacted]	1.239 1.323 [redacted]	1.195 1.387 0	0.692 0.740 [redacted]	1.178 1.366 0	1.211 1.299 [redacted]	1.278 1.373 [redacted]	1.163 1.289 [redacted]	0.887 1.175 0	0.317 0.707 [redacted]		
			0.318 0.710 [redacted]	1.028 1.453 0	1.308 1.519 0	1.208 1.310 [redacted]	1.022 1.140 [redacted]	1.051 1.173 [redacted]	1.009 1.122 [redacted]	1.191 1.299 [redacted]	1.296 1.506 0	1.022 1.444 0	0.317 0.702 [redacted]			
					0.846 1.345 0	1.100 1.441 0	1.028 1.262 0	1.219 1.448 0	1.020 1.256 0	1.088 1.425 0	0.837 1.331 0					
							0.265 0.551 [redacted]	0.320 0.617 [redacted]	0.264 0.549 [redacted]							

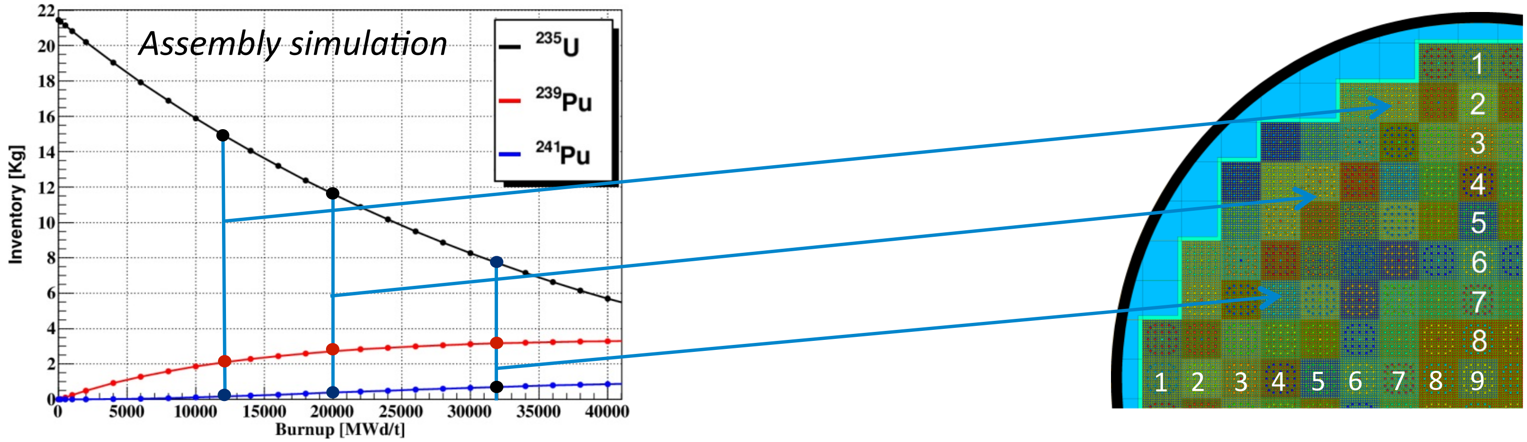
PUISSANCE MOYENNE ASSEMBLAGE
PUISSANCE MAX CRAYON
IRRADIATION ASSEMBLAGE

Each assembly is loaded in the core with a different burnup (burnup = level of irradiation).

⇒ Different initial fuel composition for each assembly at the start of a new cycle.

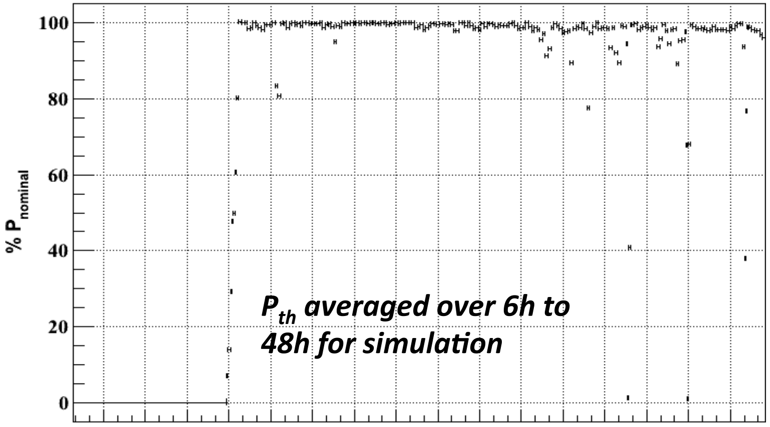
Chooz PWR core simulations

- **Initial core inventories :**
  - Individual assembly simulation with evolution until their **core loading burnup**
  - Extraction of each assembly fuel composition (Heavy nuclei & FP) and averaging to fill core simulation



Core simulation discretized into ~50 evolving cells

- **Thermal power history**



P_{th} averaged over 6h to 48h for simulation

➨ *P_{th}* Estimate through measurements of the mean temperature and flow in the 4 primary loops

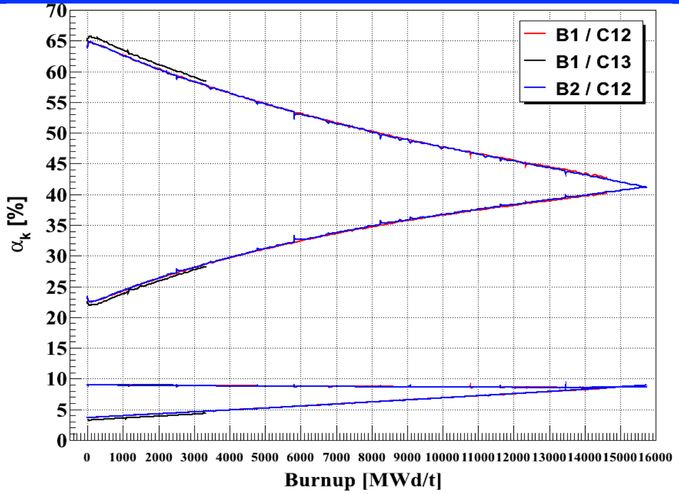
➨ Evaluated over time steps of < 1 minute

➨ **At the nominal full power of 4250 MW:**

$$\sigma_{Pth} = 0.5\% \ (1\ \sigma \text{ C.L.}).$$

A. Onillon's PhD thesis Univ. Of Nantes, France

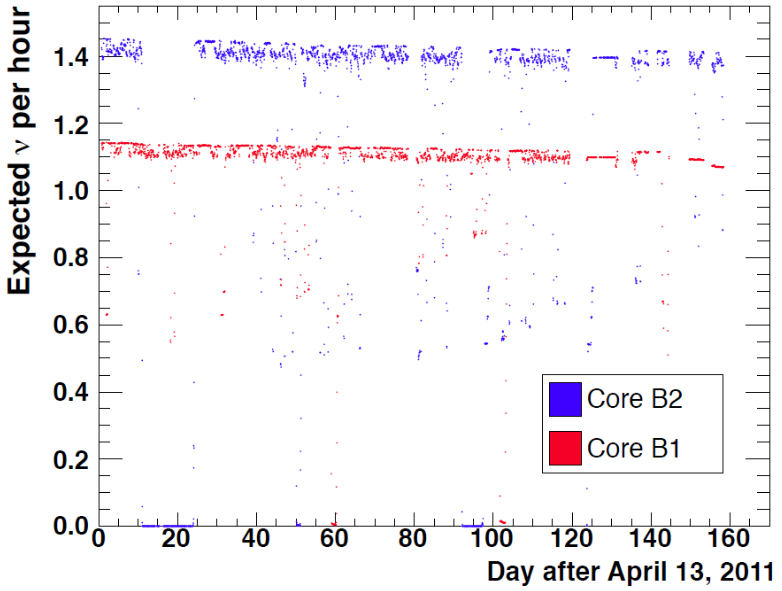
DChooz: Antineutrino flux and spectrum prediction



- Far detector data only
- No-Oscillation ⇒ reactor flux prediction via core simulations
- Normalisation to the Bugey-4 cross-section with far detector only

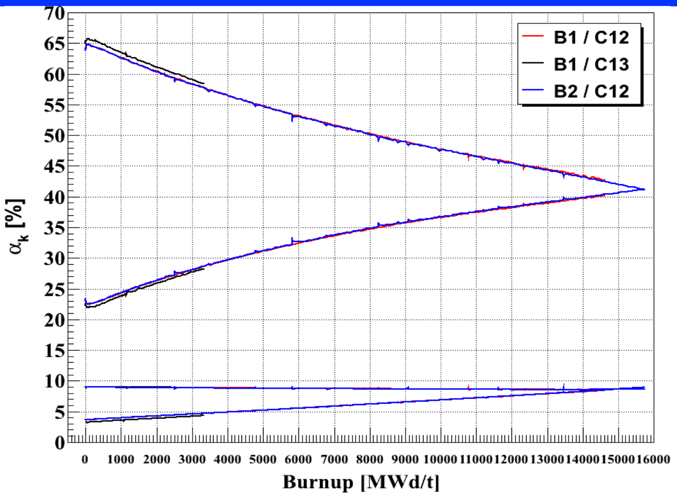
⇒ Reduced reactor systematics:

Full core simulations with the MURE code, with a follow-up of thermal power and boron concentration (>700h CPU for a complete cycle)



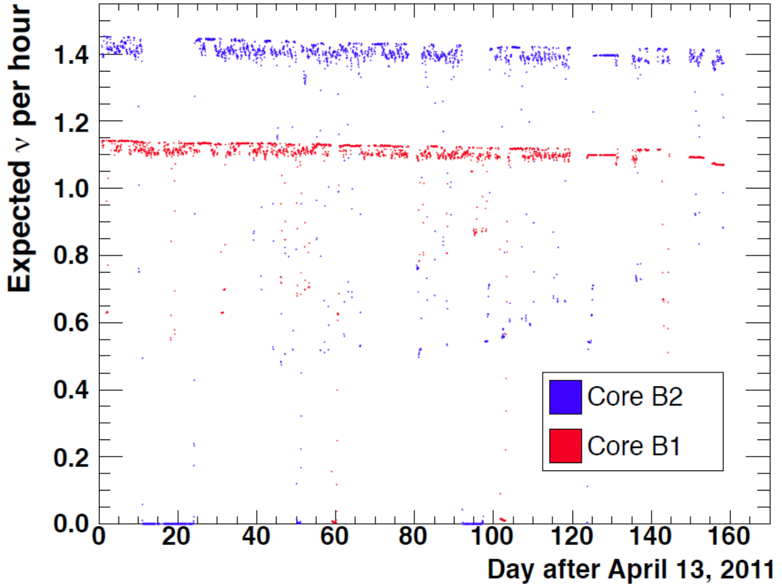
A. Onillon’s PhD thesis Univ. Of Nantes, France

DChooz: Antineutrino flux and spectrum prediction



- Far detector data only
- No-Oscillation ⇒ reactor flux prediction via core simulations
- Normalisation to the Bugey-4 cross-section with far detector only

⇒ Reduced reactor systematics:



Full core simulations with the MURE code, with a follow-up of thermal power and boron concentration (>700h CPU for a complete cycle)

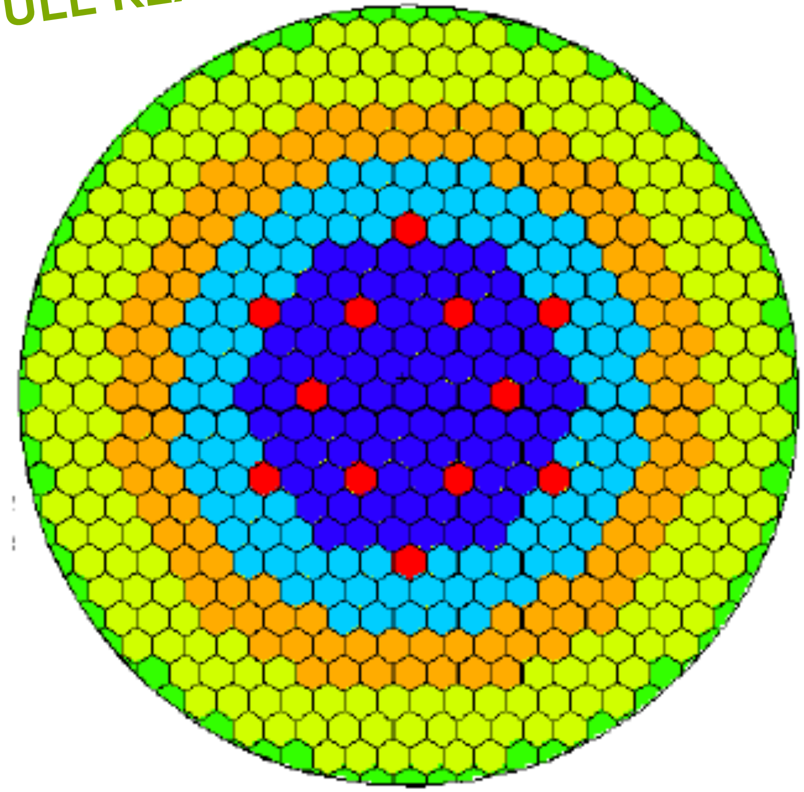
⇒ Fractions of fissions per isotope ^{235}U=49.6%, ^{239}Pu=35.1%, ^{241}Pu=6.6%, and ^{238}U=8.7% and the fission rate covariance matrix.

⇒ Numerical computation of the systematic error associated to the fission fractions with MURE over the fuel cycle: ±3.3%, ±4%, ±11.0% and ±6.5%

Total reactor error: 1.7%
Accurate reactor simulations keep the contribution of fission fraction uncertainties low

Reactor Monitoring & Nuclear Data

FULL REACTOR SIMULATION



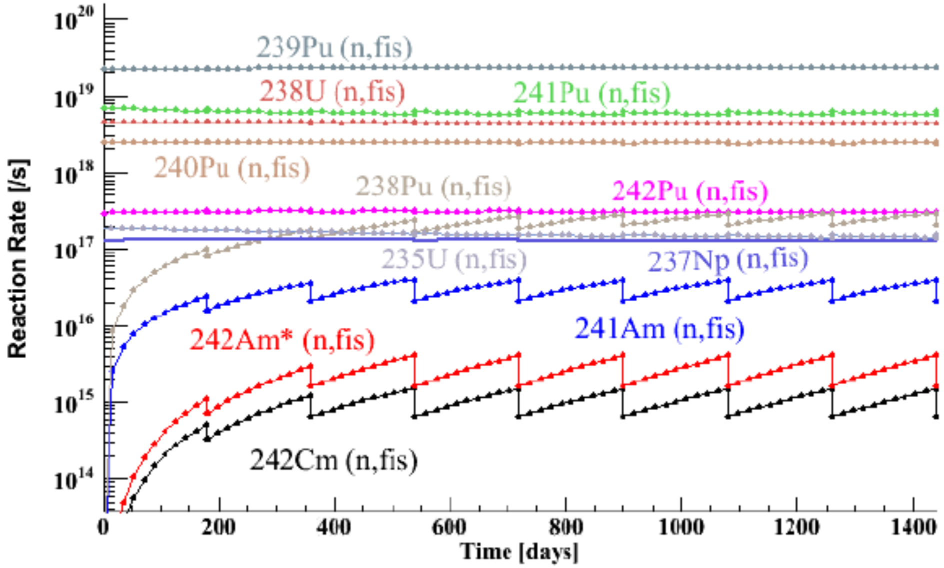
1250MWth - refuelling every 180 days
sodium-cooled
Inner core: 21% Pu, refuelled 1/3
Exterior core: 28% Pu, refuelled 1/3
Radial Blanket: MA, refuelled 1/8
Axial Blanket: MA, refuelled 1/3

Simul of reactor start-up and 8 first cycles

S. Cormon PhD thesis
http://tel.archives-ouvertes.fr/tel-00825082

- **The SM model (and thus Nuclear Data) is needed for computing antineutrino emission from future reactor designs**

Na-Fast Breeder Reactor



Several compositions of the blankets can be studied

Example of Minor Actinides (MA) composition of the blankets

Ex.: high burnup (1500 days), energy interval 4 – 5 MeV

Z	A	I	NR + MA Blankets
41	100	0	5,94272
39	96	0	5,01533
41	102	0	3,85805
52	135	0	3,68247
37	92	0	3,23426
55	142	0	3,16691
55	140	0	3,07956
53	136	1	2,95265
40	101	0	2,83245
39	98	1	2,76046
39	99	0	2,54965
53	137	0	2,32401
38	95	0	2,28268
43	108	0	1,7176
55	141	0	1,7098
39	97	1	1,59566
54	139	0	1,58208
37	93	0	1,42392
41	98	0	1,36132

In this example: most of them already measured by TAGS !!!

List of contributors extracted by M. Estienne, with SM-2017 model

Conclusions & Outlooks

- The summation method is the one allowing to predict antineutrino spectra from any reactor design or any fuel

- It requires high quality nuclear data, either decay data, shape factors or fission yields

- TAGS data measured over a decade at Jyväskylä by the Nantes-Valencia collaboration (mentioned today, see also **Algora, Tain, Rubio, Fallot, Gelletly, Eur. Phys. J. A 57, 85 (2021)**) or by our US colleagues* (shown yesterday and tomorrow) have greatly improved the agreement between the measured antineutrino flux and the summation predictions

***B. C. Rasco et al., Phys. Rev. Lett. 117, 092501 (2016), B.C. Rasco et al. Phys. Rev. C 95, 054328 (2017), A. Fijalkowska et al. Phys. Rev. Lett. 119, 052503 (2017)**

- Antineutrino energy spectra help improving the critical evaluation of nuclear data, become a powerfull tool when combined with a model such as GEF

- Need of integral antineutrino data to compare with !!!

Using Summation Method:

« With better resolution and small bin intervals, the contributions from individual nuclides, not captured in the conversion, begin to appear. Must rely on nuclear databases to understand them »

A. A. Sonzogni, M. Nino, and E. A. McCutchan PRC 98, 014323

- Did not mention here shape factors, shape anomaly, etc.

TAS COLLABORATION

IFIC Valencia: A. Algora, B. Rubio, J.A. Ros, V. Guadilla, J.L. Tain, E. Valencia, A.M. Piza, S. Orrigo, M.D. Jordan, J. Agramunt

SUBATECH Nantes: J.A. Briz, M. Fallot, A. Porta, A.-A. Zakari-Issoufou, M. Estienne, T. Shiba, A.S. Cucoanes

U. Surrey: W. Gelletly

IGISOL Jyvaskyla: H. Penttilä, Äystö, T. Eronen, A. Kankainen, V. Eloma, J. Hakala, A. Jokinen, I. Moore, J. Rissanen, C. Weber

CIEMAT Madrid: T. Martinez, L.M. Fraile, V. Vedia, E. Nacher

IPN Orsay: M. Lebois, J. Wilson

BNL New-York: A. Sonzogni

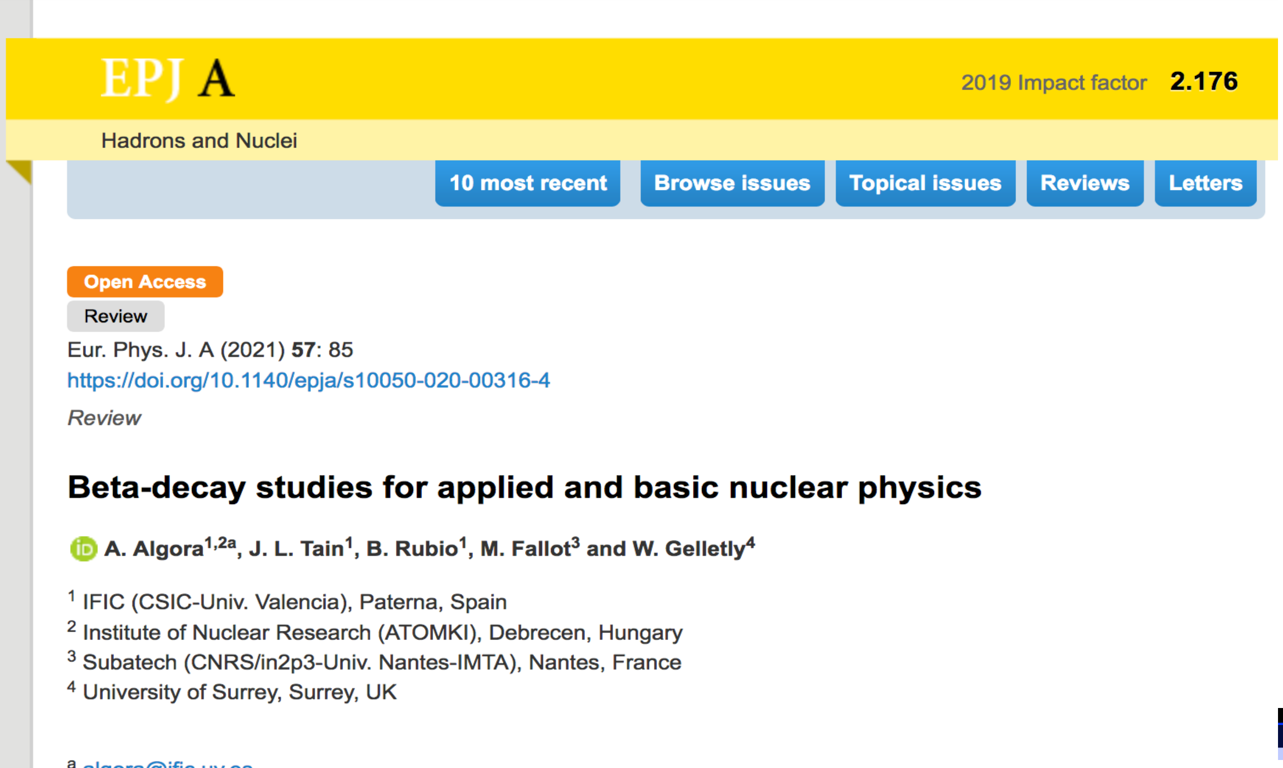
Istanbul Univ.: E. Ganioglu

Special thanks to the young researchers working in the project:
A. Beloeuvre, L. Le Meur, J.A. Briz, V. Guadilla, E. Valencia, S. Rice, A. -A. Zakari-Issoufou
Discussions with and slides from: A. Algora, J. L. Tain, B. Rubio, S. Cormon, A. Cucoanes, M. Estienne, L. Giot, A. Porta, T. Shiba, …are acknowledged

Impact of TAGS measurements over the decade

Motivations: fundamental ν physics: reactor rate & shape anomalies, reactor monitoring

- **Our Summation Model provided the priority list from IAEA-NDS Report 676**
- **14 nuclei from priority list measured in TAGS campaigns**
- **Improved Summation Method**
- **Estimated impact of inclusion of 17 published TAGS decays on reactor antineutrino spectra: 10 years of measurements**



EPJ A

2019 Impact factor **2.176**

Hadrons and Nuclei

Eur. Phys. J. A (2021) **57**: 85

https://doi.org/10.1140/epja/s10050-020-00316-4

Review

Beta-decay studies for applied and basic nuclear physics

A. Algora[1,2a], J. L. Tain[1], B. Rubio[1], M. Fallot[3] and W. Gelletly[4]

[1] IFIC (CSIC-Univ. Valencia), Paterna, Spain
[2] Institute of Nuclear Research (ATOMKI), Debrecen, Hungary
[3] Subatech (CNRS/in2p3-Univ. Nantes-IMTA), Nantes, France
[4] University of Surrey, Surrey, UK

[a] algora@ific.uv.es

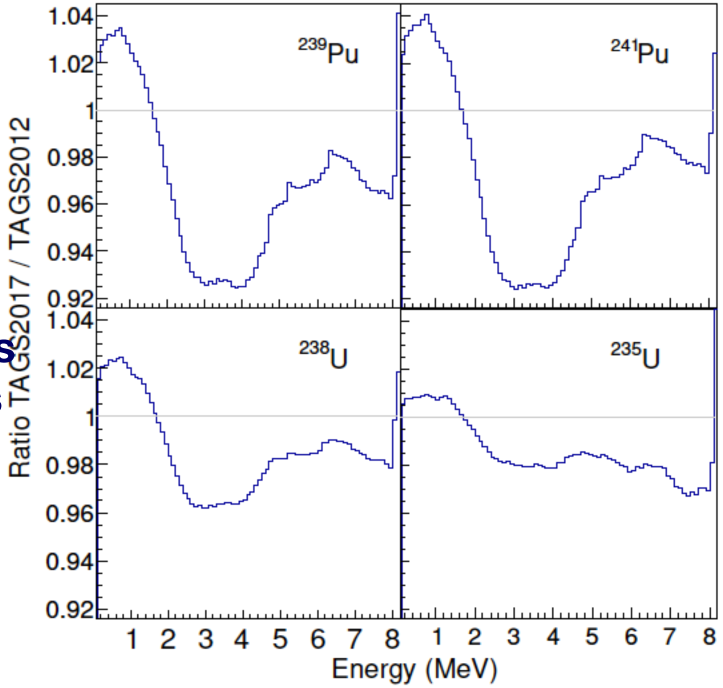


Fig. 17. Accumulated impact of the beta intensities of the ^{86,87,88}Br and ^{91,92,94}Rb [24,62,67] decays measured with the total absorption spectrometer *Rocinante* on the antineutrino spectra with respect to that published in [99] (relative ratios) for the thermal fissions of ^{235}U, ^{239}Pu and ^{241}Pu, and the fast fission of ^{238}U [107].

Review Paper: Algora, Tain, Rubio, Fallot, Gelletly, Eur. Phys. J. A 57, 85 (2021)

Impact of TAGS measurements over the decade

Motivation: decay heat released after reactor shut-down (6-12% of the nominal power), essentially radioactive decays of FP and actinides => safety & economics

- **New!** Summation Calculations with the SERPENT code:

$$\mathbf{f}(t) = \sum_i (\underbrace{\bar{E}_{\beta,i} + \bar{E}_{\gamma,i}}_{\beta,\gamma\ \text{decay}})\underbrace{\lambda_i \mathbf{N}_i(t)}_{\text{Decay constant and Fission Yield}}$$

- **Still issues with nuclear decay data**: Pandemonium Effect
- 11 new nuclei from priority list measured in TAGS campaign
- Estimated impact of inclusion of 13 published TAGS decays on Decay Heat of fission pulses

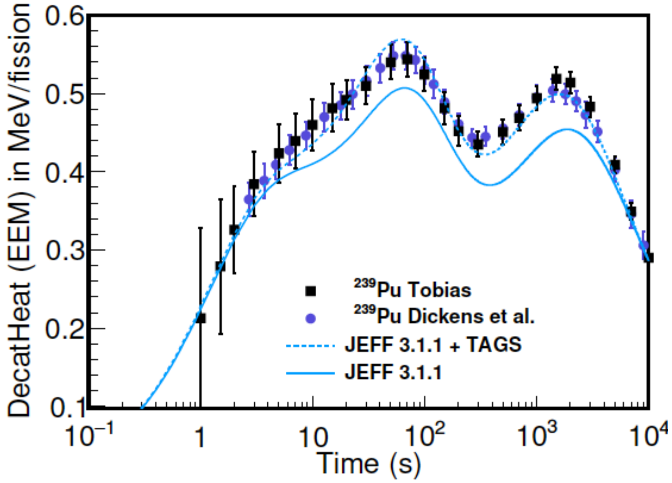


Fig. 13. Impact of the inclusion of the total absorption measurements performed for 13 decays (^{86,87,88}Br, ^{91,91,94}Rb, ^{101}Nb, ^{105}Mo, ^{102,104,105,106,107}Tc) published in Refs. [7,8,24, 62,67] in the gamma component of the decay heat calculations for ^{239}Pu.

EPJ A

2019 Impact factor **2.176**

Hadrons and Nuclei

Open Access

Review

Eur. Phys. J. A (2021) **57**: 85

https://doi.org/10.1140/epja/s10050-020-00316-4

Review

Beta-decay studies for applied and basic nuclear physics

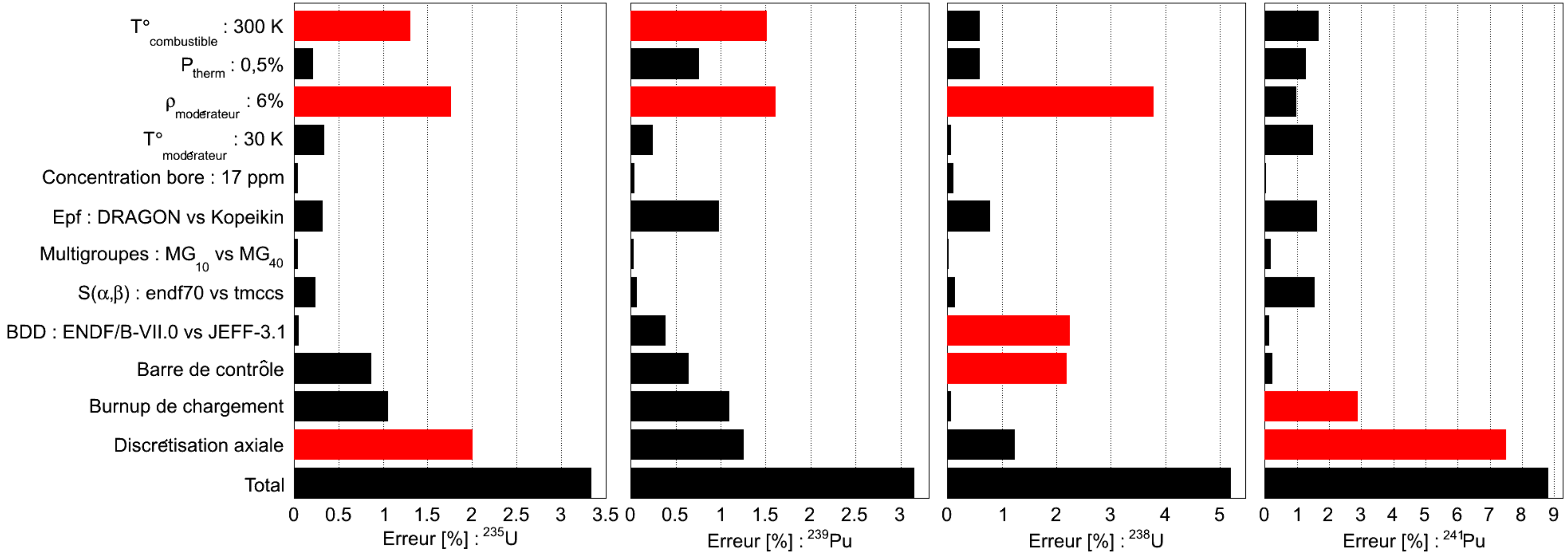
A. Algora[1,2a], J. L. Tain[1], B. Rubio[1], M. Fallot[3] and W. Gelletly[4]

Review Paper: Algora, Tain, Rubio, Fallot, Gelletly, Eur. Phys. J. A 57, 85 (2021)

Summary of the Uncertainties on the Fission Fractions

A. Onillon’s PhD, Subatech Univ. Of Nantes, https://tel.archives-ouvertes.fr/tel-01082405

Uncertainties on the total number of fissions for an irradiation cycle (B2/C12) :



	^{235}U	^{239}Pu	^{238}U	^{241}Pu
Fraction de fission [%]	$51{,}33 \pm 1{,}71$	$33{,}74 \pm 1{,}07$	$8{,}72 \pm 0{,}45$	$6{,}21 \pm 0{,}54$
Incertitudes relatives [%]	3,3	3,2	5,2	8,8

Paper in preparation…