ACORES, a software for fitting efficiency calibration curves including correlations

Boyer Bruno and Lépy Marie-Christine
Université Paris-Saclay, CEA, LIST, Laboratoire National Henri Becquerel (LNE-LNHB), F-91120 Palaiseau, France

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Introduction

- The **efficiency calibration** of a HPGe detector is an essential step before being put into service
- **Uncertainty calculations** are a major issue → direct impact on quantitative results
- **ACORES** has been developed to generate efficiency curves from experimental data **including correlations**

Calculation principle

Experimental measurements of reference sources give a series of (E, ε) pairs where E is the energy (peak position) and $\varepsilon(E)$ the full-peak efficiency given by

$$\varepsilon(E) = \frac{N(E)}{A \cdot I(E) \cdot t} \cdot \prod_i C_i$$

- $N(E)$: counts in the full-energy peak
- A: radionuclide activity (Bq)
- $I(E)$: emission intensity at energy E
- t: acquisition duration (live time) (s)
- C_i: correction factors

How to get intermediate values?
→ Fit experimental values to obtain the efficiency curve

- Models + X^2 minimization
  - APOLOG

$$ln(\varepsilon) = \sum_{k=1}^{p} a_k \cdot (ln(E))^{k-1}$$

  - APOCOPE

$$ln(\varepsilon) = \sum_{k=1}^{p} a_k \cdot (E)^{1-k}$$

  - p: degree of the fitting function
  - a_k: adjustment coefficient of order k

- **Correlations taken into account using the covariance matrix**
- Matrix formalism
  - $A_{ij} = \ln(E_i)^{j-1}$ or $(1/E_i)^{j-1}$
  - Input data vector b: $b_i = ln(\varepsilon_i)$
  - Adjustment coefficients vector

$$a = (a_1, a_2, \ldots a_p)$$

  - Covariance matrix V:

$$V_{i,j} = \left[\frac{u^2(N_i)}{N_i^2} + \frac{u^2(I_i)}{I_i^2}\right] \cdot \delta_{ij} + \frac{u^2(A)}{A^2}$$

- Solution
  - $a = [A^T \cdot V^{-1} \cdot A]^{-1} \cdot A^T \cdot V^{-1} \cdot b$
- Uncertainties
  - Coefficients: $V_a = [A^T \cdot V^{-1} \cdot A]^{-1}$
  - Calculated efficiencies: $V_\varepsilon = D \cdot V_a \cdot D^T$
    D is the matrix of derivatives of ε with respect to the parameters.

Software presentation

- First release in 1996 then updated in 2008
- Rewritten in 2025 using Python and Qt
- 2025 vs 2008 tests have been carried out

→ Upgrade validated

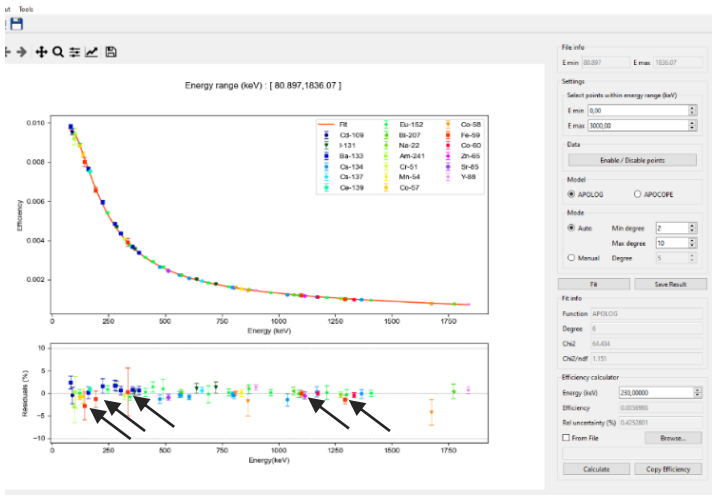
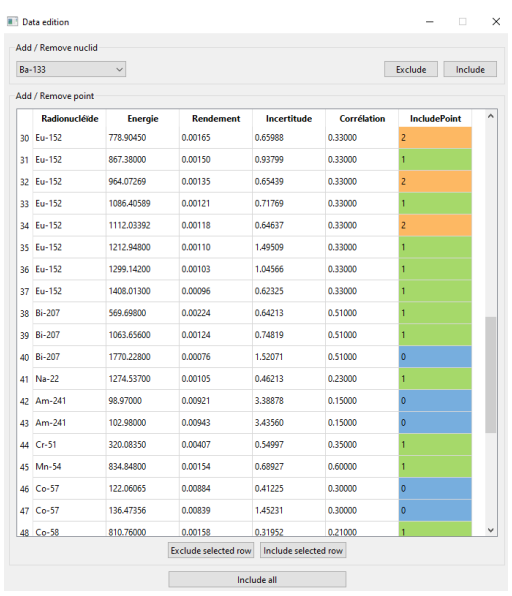


Fig. 1. ACORES GUI. Black arrows show ^{59}Fe data points

Features

- Input data: xlsx or csv file format
- Adjustable energy range
- Data editing (Fig. 2)
- Model selection: APOLOG or APOCOPE
- Auto (stops at the lowest X^2) or manual
- Result can be saved in xlsx or csv format
- Efficiency calculator: single value or multiple values from a file



	Radionucléide	Energie	Rendement	Incertitude	Corrélation	IncludePoint
30	Eu-152	778.90450	0.00165	0.65988	0.33000	2
31	Eu-152	867.38000	0.00150	0.93799	0.33000	1
32	Eu-152	964.07269	0.00135	0.65439	0.33000	2
33	Eu-152	1086.40589	0.00121	0.71769	0.33000	1
34	Eu-152	1112.03392	0.00118	0.64637	0.33000	2
35	Eu-152	1212.94800	0.00110	1.49509	0.33000	1
36	Eu-152	1299.14200	0.00103	1.04566	0.33000	1
37	Eu-152	1408.01300	0.00096	0.62325	0.33000	1
38	Bi-207	569.69800	0.00224	0.64213	0.51000	1
39	Bi-207	1063.65600	0.00124	0.74819	0.51000	1
40	Bi-207	1770.22800	0.00076	1.52071	0.51000	0
41	Na-22	1274.53700	0.00105	0.46213	0.23000	1
42	Am-241	98.97000	0.00921	3.38878	0.15000	0
43	Am-241	102.98000	0.00943	3.43560	0.15000	0
44	Cr-51	320.08350	0.00407	0.54997	0.35000	1
45	Mn-54	834.84800	0.00154	0.68927	0.60000	1
46	Co-57	122.06065	0.00884	0.41225	0.30000	0
47	Co-57	136.47356	0.00839	1.45231	0.30000	0
48	Co-58	810.76000	0.00158	0.31952	0.21000	1

Fig. 2. Data editing window

- **Point status**
  - Included
  - Excluded individually or by radionuclide
  - Excluded by energy value

Example: ^{59}Fe intensities

Discrepancy in the efficiency of the low-energy emissions (Fig. 1 ↖)

- Building the efficiency curve from the calibration dataset excluding ^{59}Fe to avoid autocorrelation (Fig. 3)

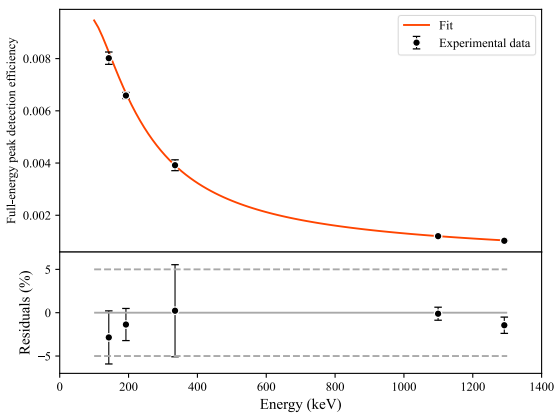


Fig. 3. ACORES efficiency curve

- ACORES & $I(E) = \frac{N(E)}{A \cdot \varepsilon(E) \cdot t} \cdot \prod_i C_i$

→ Absolute emission intensities (Fig. 4)

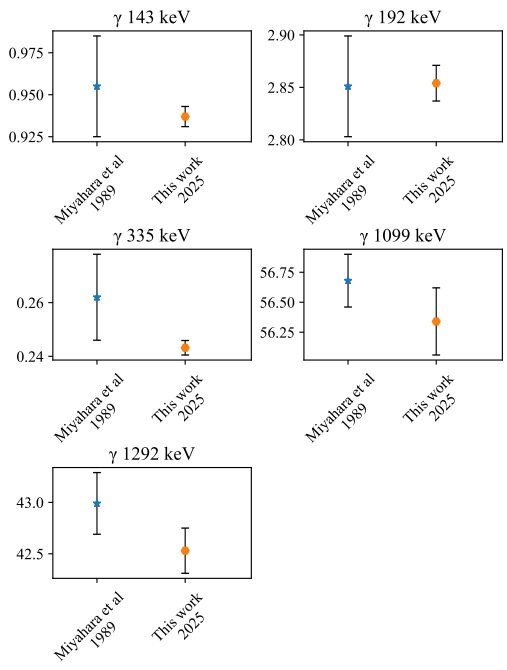


Fig. 4. ^{59}Fe absolute emission intensities

→ Agreement with Miyahara, *et al.*

Miyahara *et al.*, Appl. Rad. Isotopes - 1989 - Vol. 40 - p. 343

Relative intensities
→ Agreement with DDEP values, see the associated article

Conclusion & Outlook

- New version validated
- Knowledge of the efficiency curve
- Preliminary emission intensities of ^{59}Fe
- **Online version will be developed**