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Monte Carlo benchmark on coincidence summing corrections
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Contribution of Uncertainty of Decay Data and of the Uncertainty of the Dead Layer to the Uncertainty of Coincidence Summing Corrections

Octavian Sima
Physics Department, Univ. of Bucharest, IFIN-HH & ELI-NP, Bucharest
Romania

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1. Coincidence summing corrections – general considerations

Coincidence summing corrections for a peak of energy E_i result from:

- *Coincidence losses* due to simultaneous detection of other photons E_j
  - Proportional with joint emission probability of the E_i and E_j photons p_{ij} and with the probability of simultaneous detection of E_i in the peak and of E_j in the total spectrum
- *Coincidence summing in* in the case when the transition in which E_i is emitted can also be realized by successive transitions of photons E_p and E_q
  - Proportional with joint emission probability of the E_p and E_q photons p_{pq} and with the probability of simultaneous detection of both E_p in the peak and of E_q in the peak

In the case of a point source and negligible angular correlations:

$$F_C(E_i;X)=1-\sum_j \frac{p_{ij}}{p_i}\cdot\eta(E_j)+\sum_{j,k}\frac{p_{ijk}}{p_i}\cdot\eta(E_j)\cdot\eta(E_k)-\ldots$$

$$+\sum_{p,q}\frac{p_{pq}}{p_i}\cdot\frac{\varepsilon(E_p)\cdot\varepsilon(E_q)}{\varepsilon(E_i)}-\sum_{p,q,r}\frac{p_{pqr}}{p_i}\cdot\frac{\varepsilon(E_p)\cdot\varepsilon(E_q)\cdot\eta(E_r)}{\varepsilon(E_i)}+\ldots$$

p_i – emission probability of the E_i photon of nuclide X

p_{ij}, p_{ijk} – joint emission probability of photons E_i and E_j, respectively E_i, E_j, E_k

$\varepsilon(E)$ – full energy peak efficiency for the photon of energy E
$\eta(E)$ – total efficiency for the photon of energy E
Note:

- In the case of volume sources, the detection efficiencies for group of photons are more involved (angular correlations are neglected):

$$\varepsilon(E_i) \cdot \eta(E_j) \to \frac{1}{V}\int_V \varepsilon_P(E_i,\vec{r}) \cdot \eta_P(E_j,\vec{r})dv$$

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$\varepsilon_P(E_i,\vec{r})$ and $\eta_P(E_j,\vec{r})$ = peak and total efficiency for a point source at $\vec{r}$ (Sima & Arnold, ARI 53 (2000) 51)

2. Dependence on decay data parameters

F_C depends on decay scheme parameters through the joint emission probabilities

p_{ij}, p_{ijk} depend not only on p_i, p_j, p_k, but also on:

- Relative de-excitation of the initial level on other levels
- The conversion coefficients α_K, α_L, α
- The decay branch on each level
- ω_K in the case when X-rays contribute (K X rays fluorescence yield)
- P_K in the case of EC decays (probability of electron capture on K atomic shell)

$\Rightarrow$ The explicit dependence of p_{ij}, p_{ijk} on the decay scheme parameters: very complex in the general case

$\Rightarrow$ How to evaluate the uncertainty of F_C due to the uncertainties of the parameters of the decay scheme?

- Uncertainty propagation formula not convenient – nonlinear, correlations
- Standard Monte Carlo not convenient – decay scheme simulation mixed with radiation transport => the distribution of F_C values would have inseparable contributions both from the uncertainty of decay parameters and of radiation transport

3. Procedure for the evaluation of random decay schemes

Proposed solution (Sima & Lepy, ARI 109 (2016) 493):

- Disentangle (cf. Eq. 1) evaluation of joint emission probabilities from efficiencies (radiation transport)
- Evaluate the required joint detection probabilities (group efficiencies) by a separate, long run Monte Carlo simulation
- Prepare a large set of decay scheme data on the basis of the parameters of the decay scheme and of their uncertainties
  - data source: DDEP (http://www.nucleide.org/DDEP_WG/DDEPdata.htm)
  - p_i, P_K, ω_K – independent Gaussian distributions
  - α_K, α_L, α: two procedures: totally correlated Gaussian, or each extracted independently from a Gaussian distribution
  - Transition probabilities: from p_i and α's
  - Decay branches: probability balance (de-excitation and feeding)
  - Acceptance checks
- For each decay scheme from the set evaluate each of the necessary p_i, p_{ij}, p_{ijk} – (Sima & Arnold, ARI 66 (2008) 705)
- Using the pre-computed joint detection probabilities, for each decay scheme evaluate F_C (Eq. 1)
- Analyze the distribution of the set of F_C values: average, standard deviation

4. Results – Contributions of the uncertainty of decay scheme parameters

Computations: all the cases from the F_C benchmark exercise (2 detectors, 4 geometries, 11 peaks = 208 cases)

Generally very low uncertainties: 151 cases from 208 with uncertainty < 0.1%

Highest F_C uncertainties: detector B, point source, then detector B, filter
79 keV (B, point): 8.2%
160 kev (B, point): 4.6%
79 keV (B, filter): 4.3%

Uncertainty for F_C at 79 keV dominated by the uncertainty of p_i for 79 keV:
2.63 (19) (DDEP)

Uncertainty of p_i*F_C
- This quantity is required for activity computation using the count rate N ($N=\varepsilon_0*F_C*p_i*A$)
Higher uncertainty than for F_C !
112 from 208 cases with uncertainty < 0.5%
For 80 keV: between 1 and 1.7%

5. Conclusions – effects of decay scheme uncertainties

Generally the effect of decay scheme uncertainties on the uncertainty of coincidence summing correction factors F_C is lower than the contribution of other sources of uncertainty

- In particular cases it is not negligible – low intensity peaks with high coincidence summing from other photons

Realistic evaluation of the contribution of decay scheme uncertainties to F_C:

- Decouple evaluation of joint emission probabilities from radiation transport
- Prepare sets of random decay schemes based on Monte Carlo simulation of decay scheme parameters
    - In absence of covariance matrices of the parameters, sampling of the parameters should be arranged in line with the procedure of parameters evaluation
    - For each decay scheme evaluate the set of joint emission probabilities
    - Using fixed, independently computed, detection probabilities of groups of photons, evaluate F_C
    - Analyse the statistics of F_C distributions

6. Dead Layer problems in F_C evaluation

At low energy (< 100 keV):

- Dead layer (DL) thickness – essential for peak efficiency (high attenuation of low *E* photons in DL)
- Dead layer also important for total efficiency for low *E* photons
- Best value of the DL thickness: trial and error based on comparison of peak efficiency from simulations with measured values at low energies

At higher energies:

- Attenuation of photons in the dead layer less important
- Effect of DL on efficiency at higher energies: mainly due to the dependence of the volume of the sensitive region on DL thickness

Additional dependence on DL thickness in the case when coincidence summing effects are important (Arnold & Sima, ARI 60 (2004) 167)

$\Rightarrow$ Impact of DL thickness on apparent peak efficiency $\varepsilon(E)$ for higher energy photons: higher than expected for energy *E* in the case when coincidence summing with low energy photons is significant for the peak of energy E

  $\Rightarrow$ The effect is dominated by the attenuation of the coincident low energy photons

Measurements in PTB (Arnold & Sima, ARI 60 (2004) 167):

- Ba-133 and Eu-152 point sources with two detectors (p and n-type)
- For each detector and source:
    - One measurement with a stainless steel absorber of 0.97 mm
    - One measurement without absorber
- DL thickness evaluated by comparison simulation vs. measurement of peak efficiency at low energy ("conventional dead layer thickness")

Results:

- p-type detector:
    - Peak shape distorted in the case of measurement without absorber
        - Tail in the high energy part of the peaks affected by coincidences with X-rays (Ba-133 peaks and Eu-152 peaks from EC decay branch)
    - Computed F_C values for these peaks in disagreement with measured values if the conventional DL thickness is used in calculations
    - No problems in the case of measurements with the absorber
- n-type detector: no problems

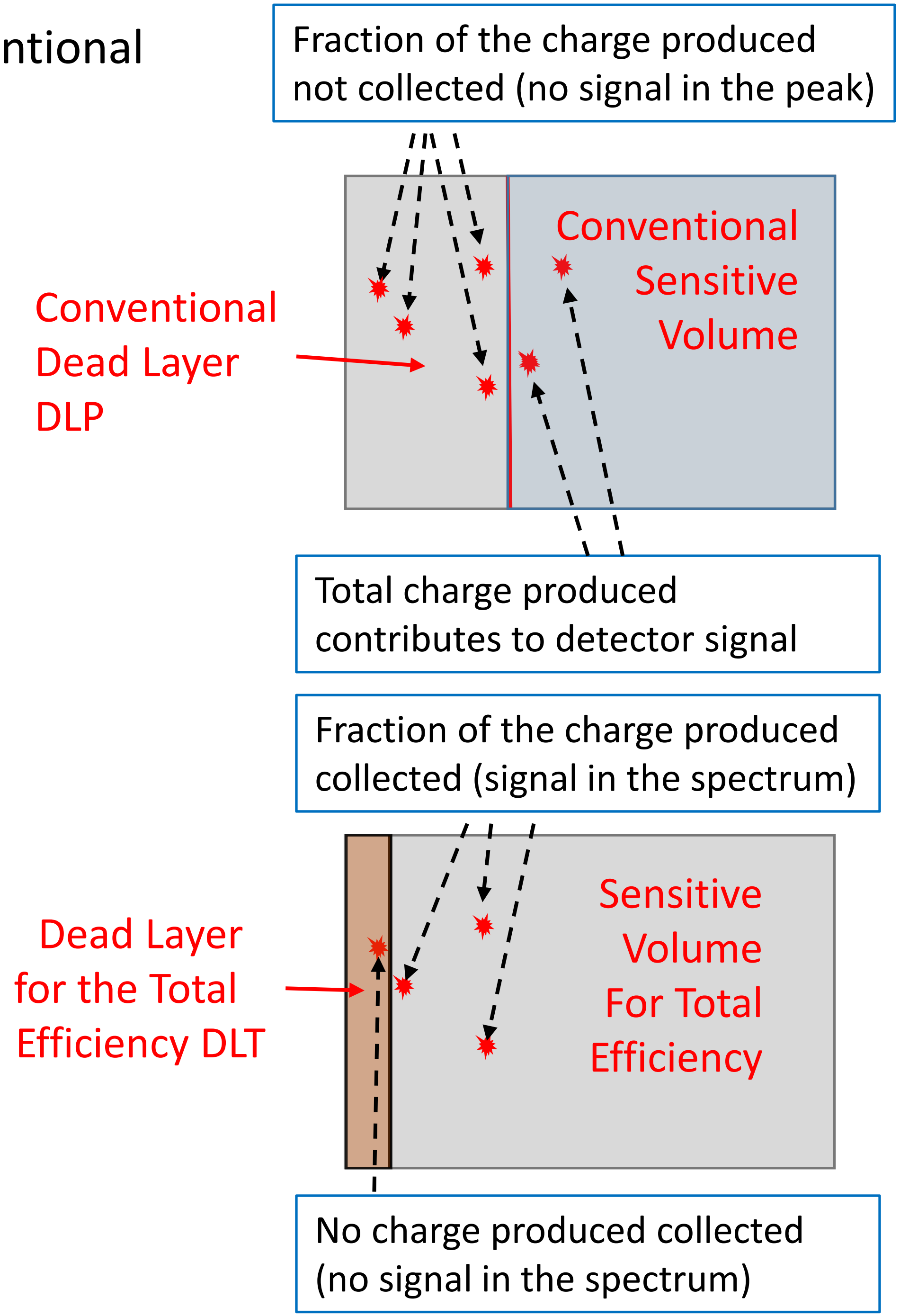
Simulations with GEANT3 and PENELOPE do not explain the distortion of the peak shape (Stancu et al., Rom. Rep. Phys. 67 (2015) 465).

Why F_C and η evaluation using conventional dead layer thickness fails?

- The sensitive volume for peak efficiency differs from the sensitive volume for total efficiency (and for coincidence losses from a peak)
- Conventional sensitive volume: all charges produced are collected
- Sensitive volume for total efficiency: some charge is collected
- Sensitive volume for total efficiency bigger than sensitive volume for peak efficiency

$\Rightarrow$ Dead layer thickness **DLT < DLP**

Difficult to measure DLT
=> Usually total efficiency and coincidence losses from peaks are evaluate using DLP (much easier to measure) instead of using DLT



7. Consequences of different dead layers for peak and total efficiency

$\Rightarrow$ Effect of DLT<DLP on the computation of the total efficiency:

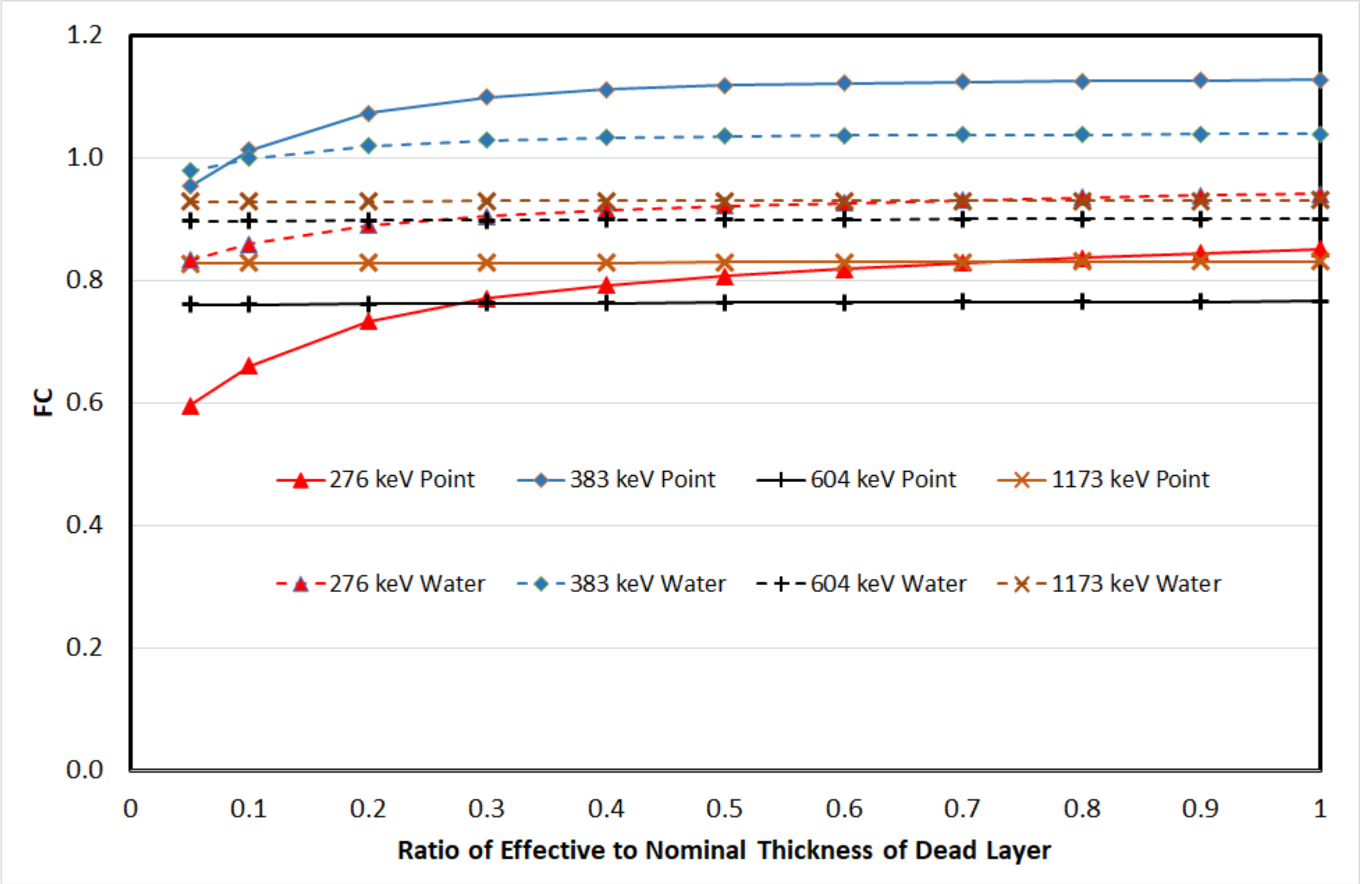
- η computed using DLP is underestimated – at high energy only due to smaller active volume when using DLP

Effect of DLT<DLP on the computations of F_C:

- Coincidence summing losses computed using DLP are underestimated
- In the case of high contribution to coincidence losses due to low energy photons, the effect on F_C is controlled by the dependence on DLT of the sensitive volume for the low energy photons
  - Losses from the peaks of higher energies E more important than the dependence of $\eta(E)$ on DLT
- In the case when only high energy photons contribute to coincidence losses, the effect of DLT<DLP less important

PTB Measurements (Arnold & Sima, ARI 60 (2004) 167):
=> Best results of F_C evaluation for Ba-133 peaks measured with the p-type detector without absorber: DTL/DLP=0.13

Calculations with GESPECOR for point and water sources (as in Benchmark…)
Detector A with nominal dead layer thickness DLP and various effective DLT values



For peaks with low energy photon coincidence summing effects: 15-20 % effect for point source, 5 % for water source

For peaks without low energy photon summing – negligible effect

=> Good knowledge of the structure of the dead layer required !

8. Conclusions – dead layer problem

- The dead layer has a complex structure
  - ⇒ The sensitive volume for peak efficiency differs from the sensitive volume for total efficiency
  - ⇒ With standard Monte Carlo simulations, in which the signal is completely related to the charge produced in the sensitive volume, it is impossible to reproduce simultaneously the peak and total efficiency, respectively the peak efficiency and the coincidence summing correction factors using a single dead layer.
  - ⇒ The distortion of the peak shape due to coincidences with low energy photons (Arnold & Sima, ARI 60 (2004) 167) cannot be reproduced by standard Monte Carlo simulations (Stancu et al., Rom. Rep. Phys. 67 (2015) 465).
- Realistic solution of the problem: include the simulation of charge collection processes in the software for detector simulation
  - Difficulties: requires knowledge of the electric field distribution, of the impurities distribution, of the charge mobility
- Practical solution: Inclusion of 2 different dead layers in simulations:
  - Conventional dead layer DLP (fixed by peak efficiency measurement at low E)
  - Dead layer for total efficiency DLT, with DLT<DLP
  - DLT may be fixed by comparison of simulations with measurements of F_C for coincidence losses due to low energy photons