LSQ and NNLSQ methods for data evaluation & Comparison of ISO 11929 and Currie MDA for Extended WND method

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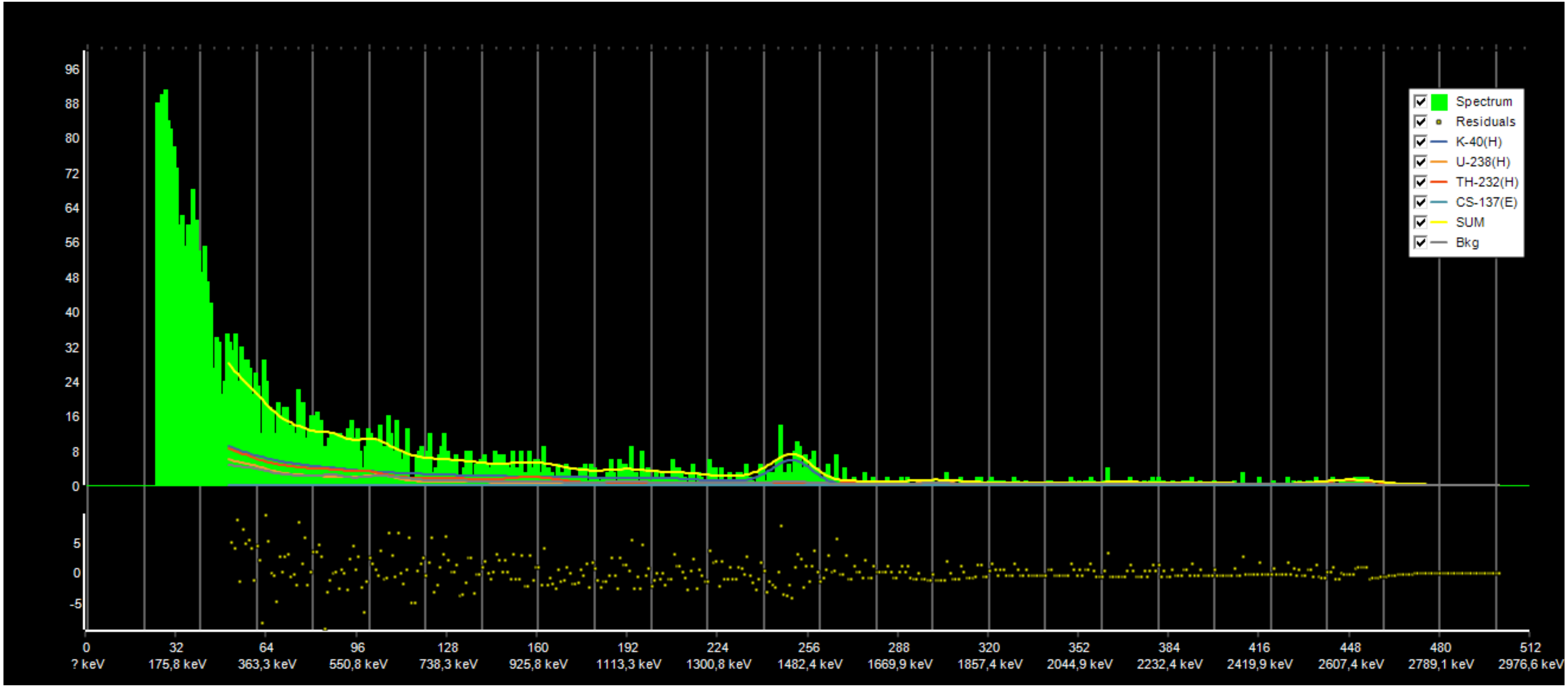
LSQ and NNLSQ methods for data evaluation

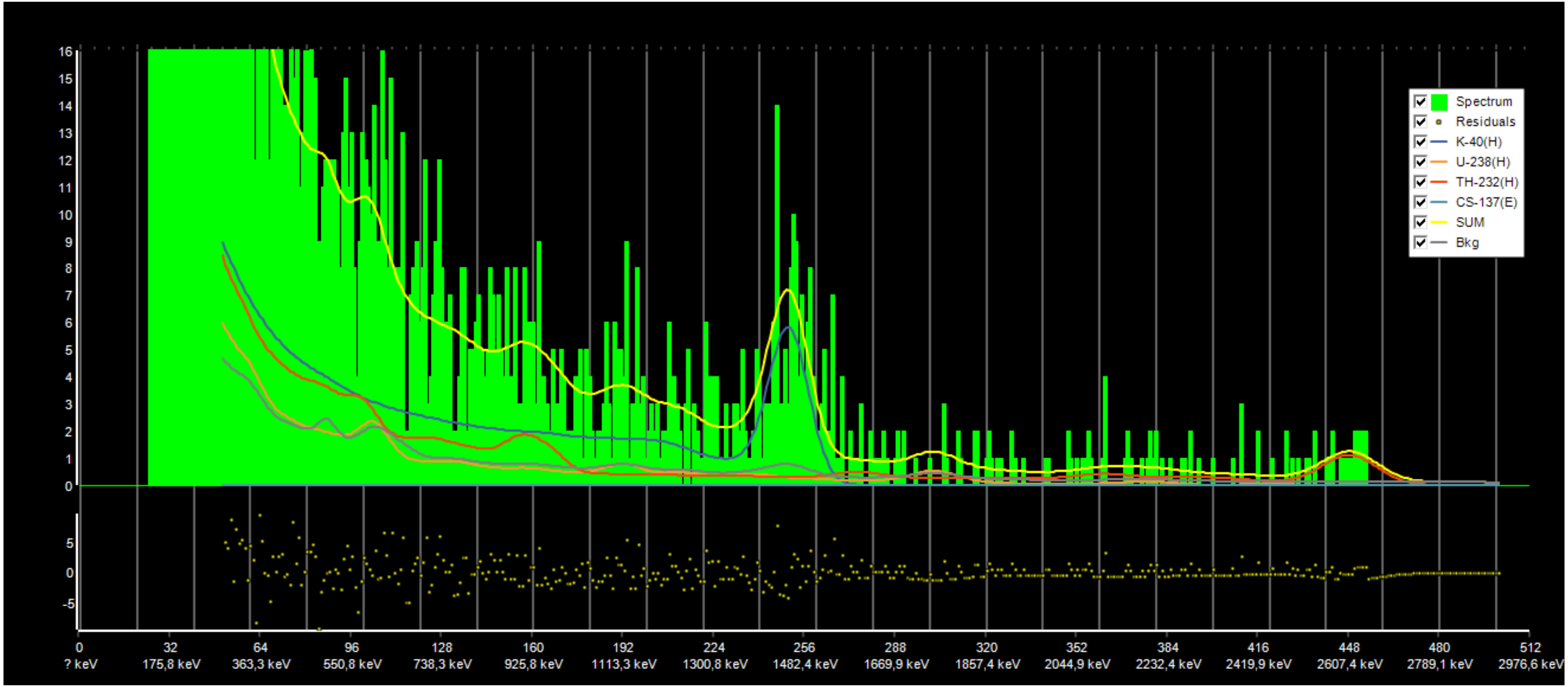
- Least squares (LSQ) – general notes
  - standard approach in regression analysis to approximate the solution of overdetermined systems
  - i.e., sets of equations in which there are more equations than unknowns
  - "Least squares" means that the overall solution minimizes the sum of the squares of the residuals made in the results of every single equation
- Our case – airborne gamma-ray spectra
  - For each measured spectrum, we are looking for activities of all four nuclides (Act_Cs, Act_K, Act_U, Act_Th)
  - We know response matrixes for each nuclide (includes efficiencies, altitude corrections, …), therefore we can write our problem as following:

  - Channel_1 [CPS] = Act_Cs * Matrix_Cs_1 + Act_K * Matrix_K_1 + Act_U * Matrix_U_1 + Act_Th * Matrix_Th_1
  - Channel_2 [CPS] = Act_Cs * Matrix_Cs_2 + Act_K * Matrix_K_2 + Act_U * Matrix_U_2 + Act_Th * Matrix_Th_2
  - ..
  - Channel_512 [CPS] = Act_Cs * Matrix_Cs_512 + Act_K * Matrix_K_512 + Act_U * Matrix_U_512 + Act_Th *Matrix_Th_512

LSQ and NNLSQ methods for data evaluation

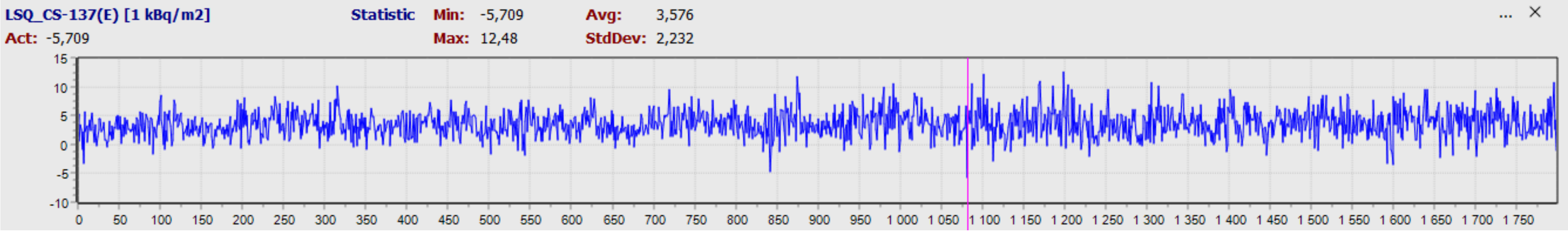


LSQ and NNLSQ methods for data evaluation



LSQ and NNLSQ methods for data evaluation

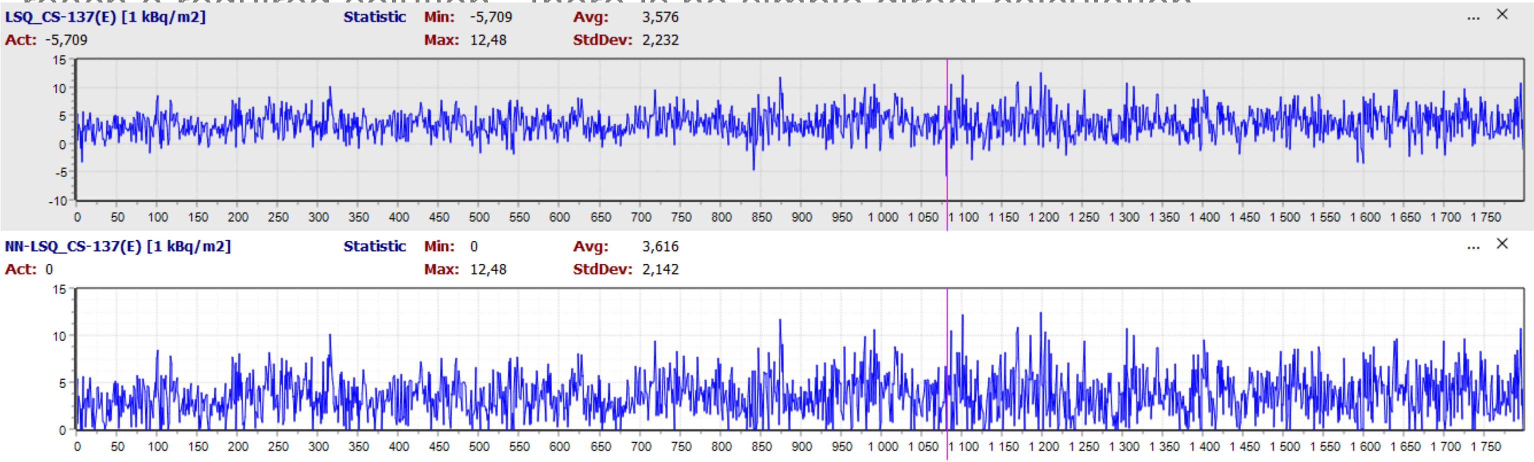
- This leads to well-known LSQ formulas, which give us estimates of required activities
- However, sometimes we obtain results, where one or more estimates are negative



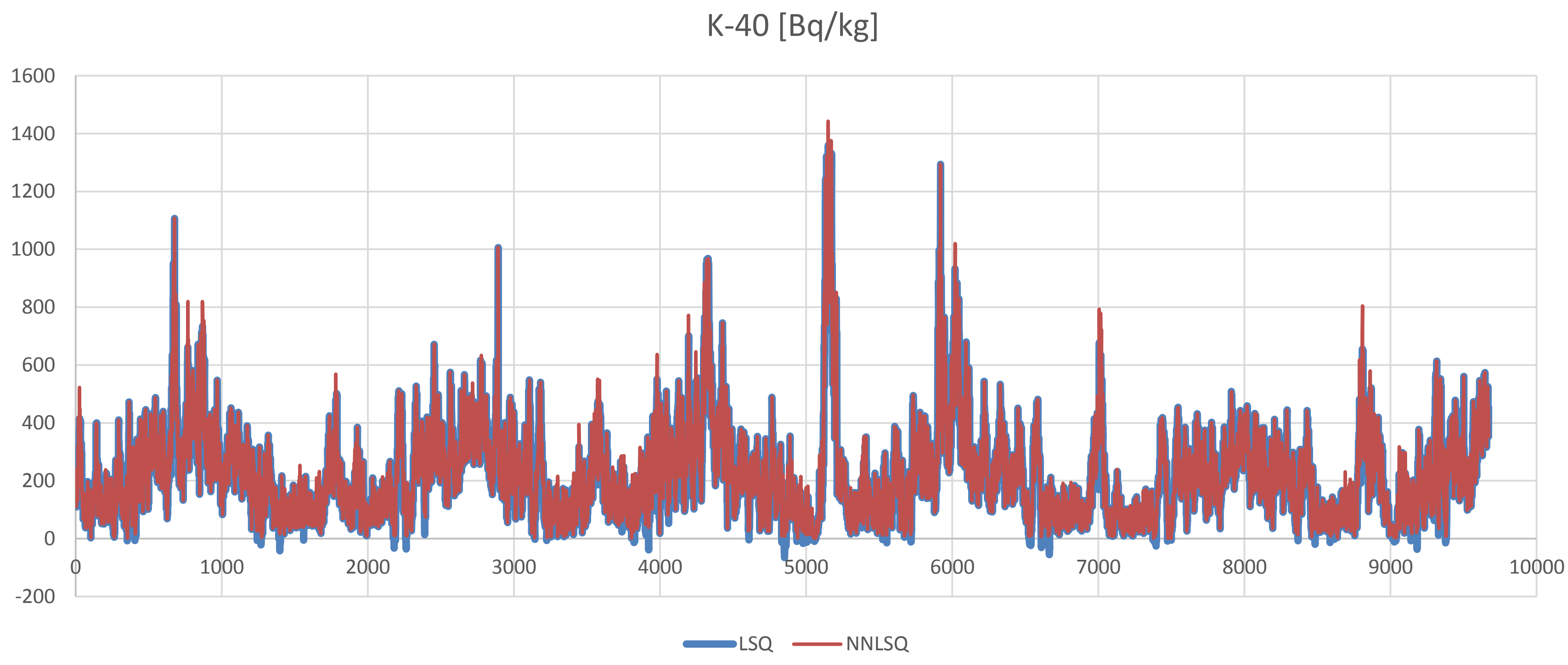
- Is it normal? – from statistical/mathematical point of view YES, from physical point of view NO
- LSQ is „searching“ for global solution in the domain of all real numbers
- What to do? Overwrite negative estimate by zero? – NO! Let‘s try NNLSQ…

LSQ and NNLSQ methods for data evaluation

- NNLSQ (non-negative least squares)
  - Type of constrained LSQ problem where the coefficients are not allowed to become negative
  - If any coefficient estimated by normal LSQ is negative, then NNLSQ is used to find new solution in the domain of positive real numbers
  - NNLSQ is done by using a specific numerical algorithm with a finite number of steps to reach a required solution – there is no simple direct calculation



LSQ and NNLSQ methods for data evaluation



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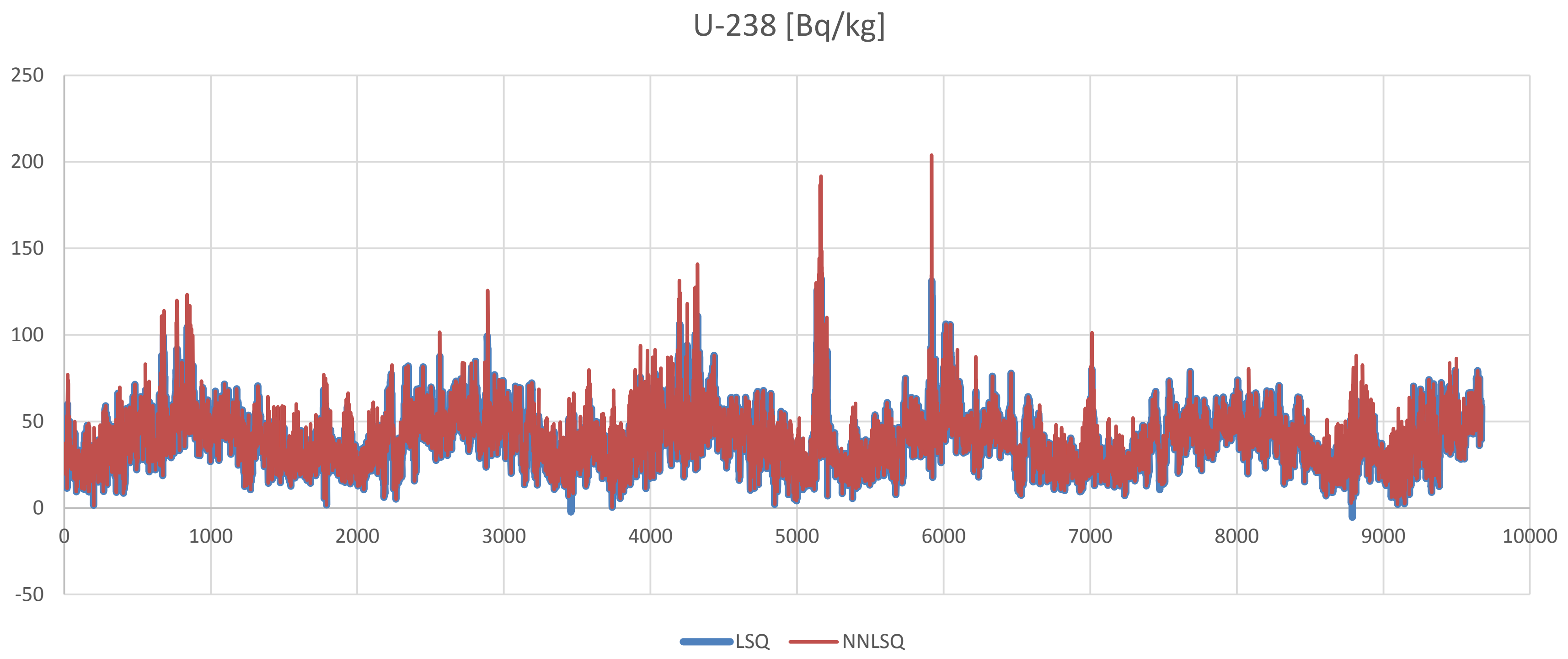

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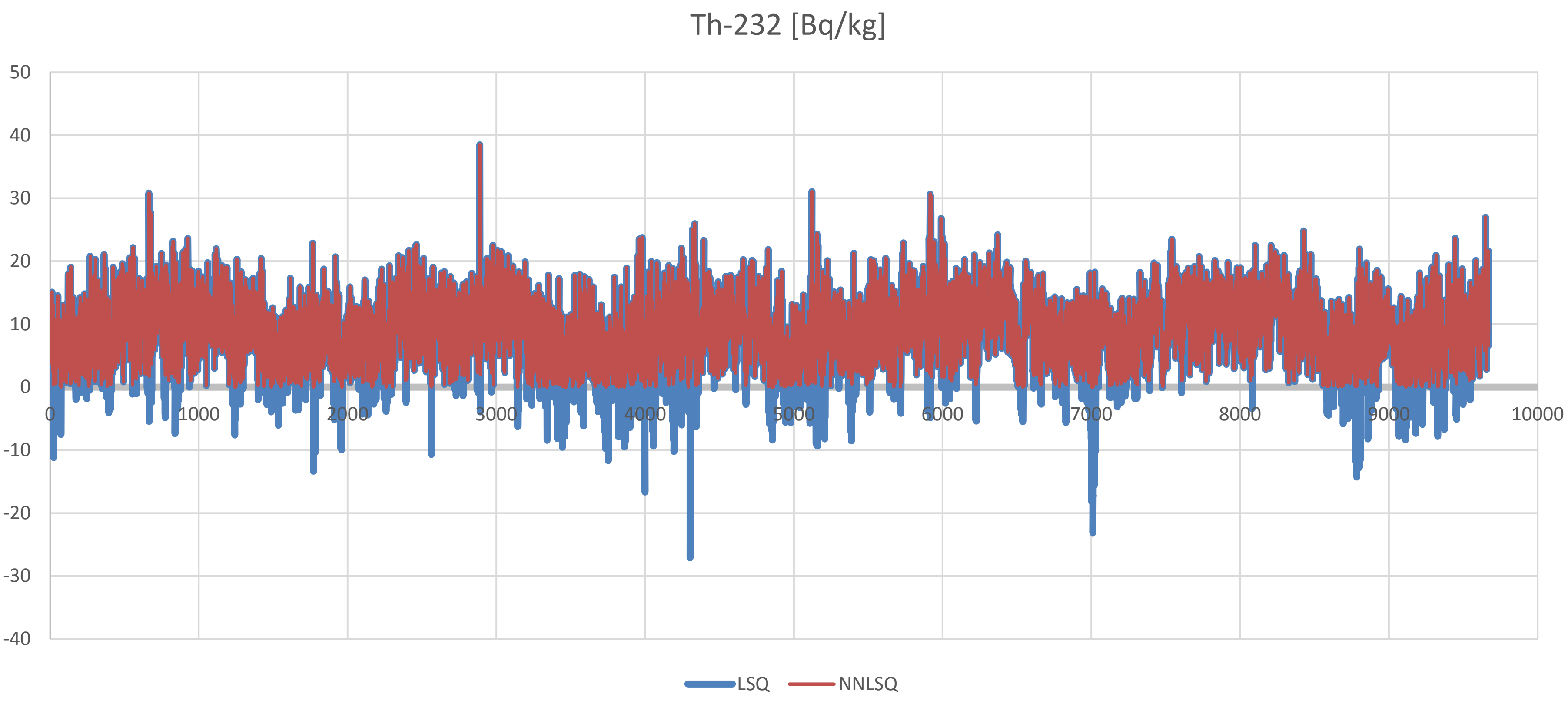

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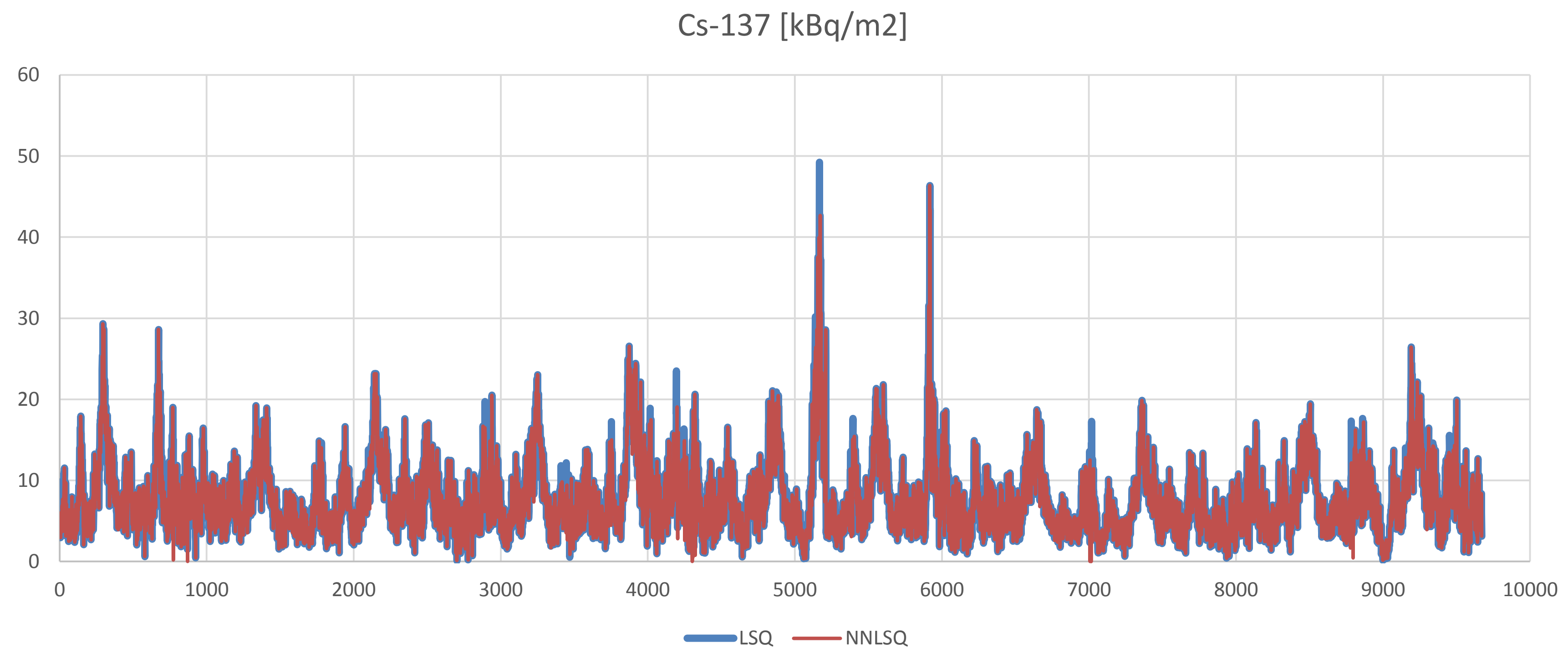
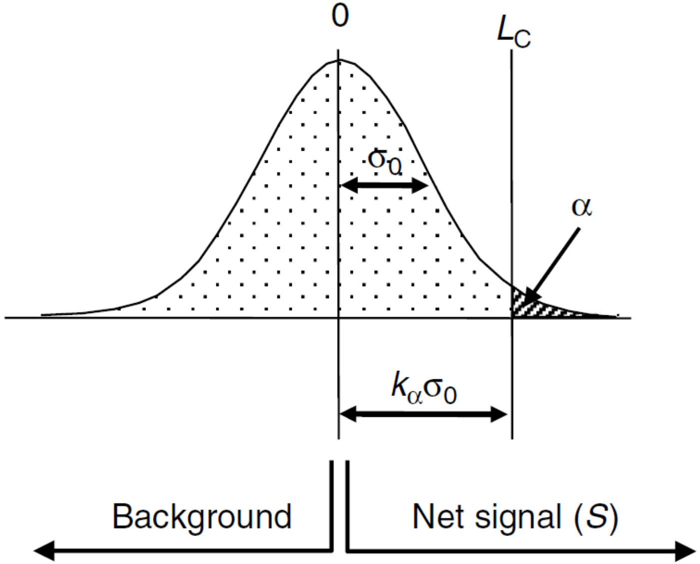


Conclusion

- NNLSQ is special modification of normal LSQ
- NNLSQ gives us a correct values of LSQ from physical point of view
- NNLSQ is performed only if normal LSQ gives negative values
- Even if only one estimated coefficient is negative, then following NNLSQ calculation can modify all other estimated coefficients (it is not changing just the negative ones)

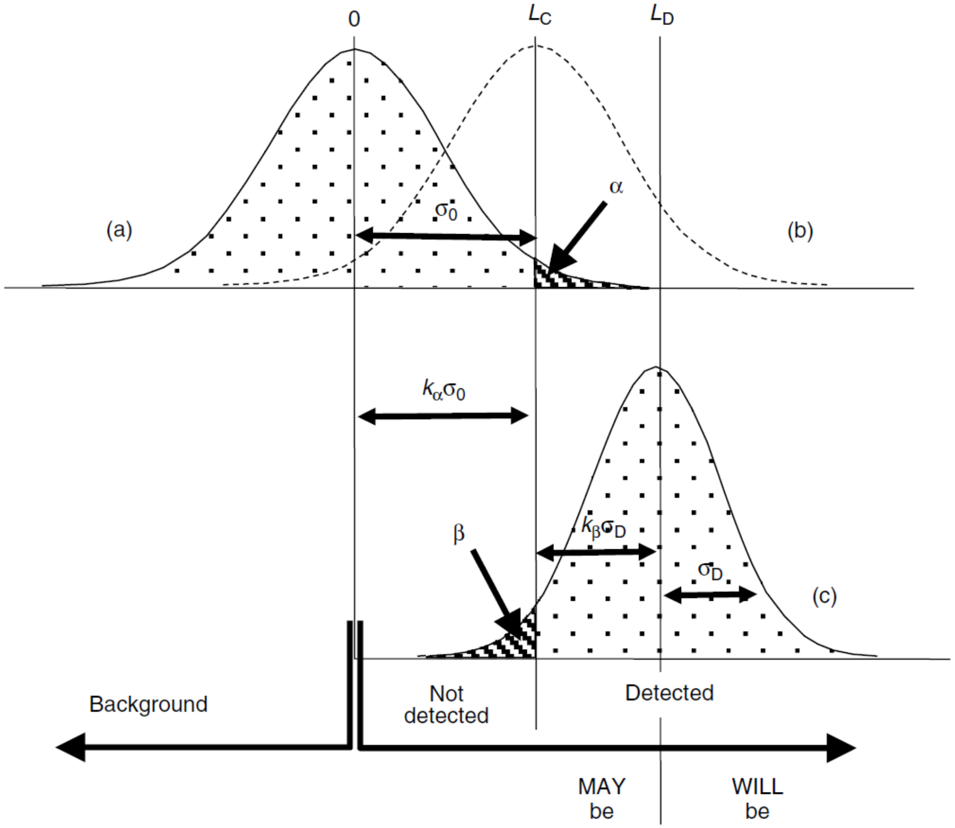
- NNLSQ is not simple to calculate manually, but it is already implemented in AGAMA SW

- Counting detections limits
  - **Critical limit** (LC) – a decision level: *'Is the net count significant?'*
  - **Minimum significant activity** (MSA) - a decision level: *'Is the activity significant?'*
  - **Detection limit** (LD) – *'What is the minimum number of counts I can be confident of detecting?'*
  - **Minimum detectable activity** (MDA) – *'What is the least amount of activity I can be confident of detecting?'*



Comparison of ISO 11929 and Currie MDA for Extended WND method

- Counting detections limits
  - (a) Activity = 0
  - (b) Activity = MSA
  - (c) Activity = MDA



Comparison of ISO 11929 and Currie MDA for Extended WND method

- Traditional "Currie MDA" calculation for net counting
  - Net_counts = Gross_counts – Background_counts
  - Requires input data with Poisson distribution -> **σ** (counts) = SQRT(counts)
  - Then by direct calculation, following formulas can be derivated (for α = β = 5 %)

LC=2.33 * SQRT(Background_counts)

LD = 2.71 + 4.65 * SQRT(Background_counts)

- New ISO 11929 Standard concept
  - General approach to obtain MDA formula for any system / algorithm
  - It gives just „step – by – step guide", the MDA formula derivation has to be done by yourself
  - Does not require only inputs with Poisson distribution
  - However, this can lead to very complicated formulas (even without explicit solution), therefore in many cases the MDA has to be found numerically

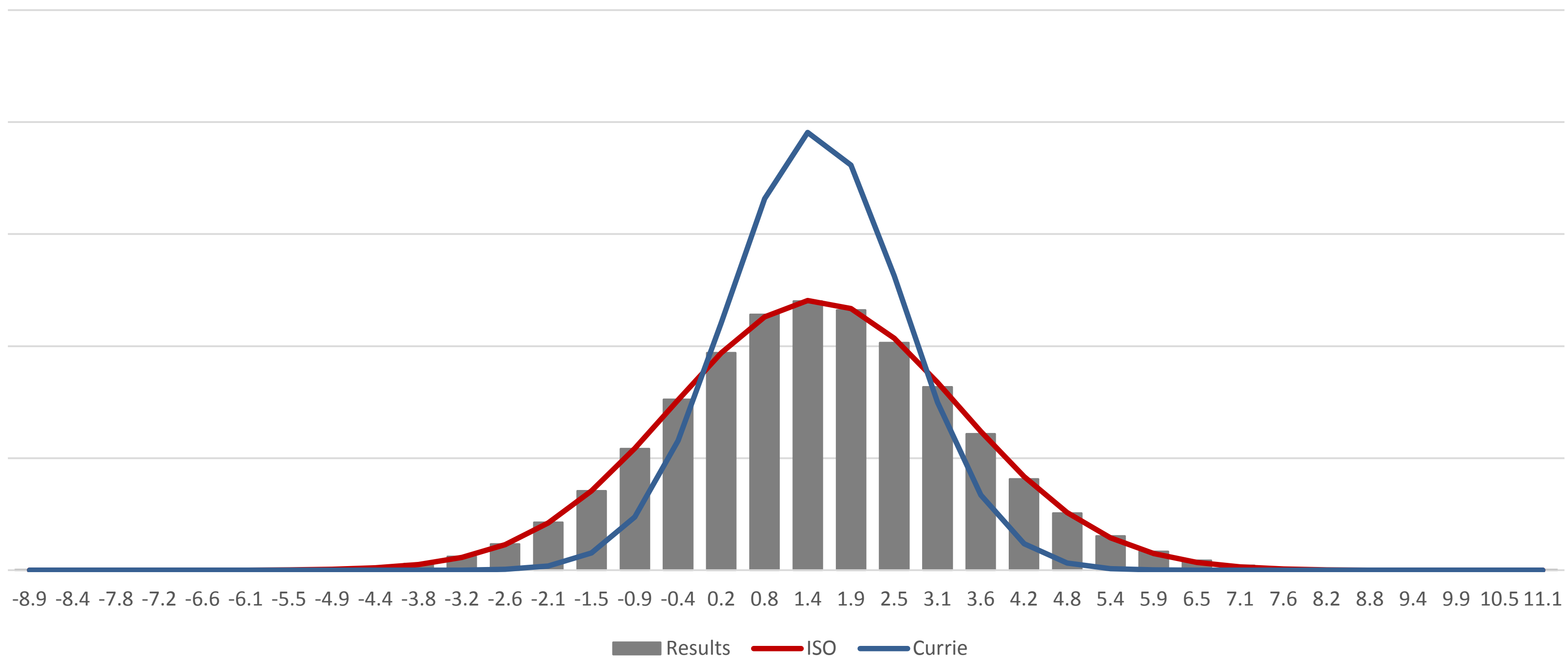
Comparison of ISO 11929 and Currie MDA for Extended WND method

- Our case – Extended WND method
  - Is WND simple „net counting“ case? – NO
  - We can try to reduce this to a simple net counting (for each nuclide) by estimating background as

    Background_counts = Net_counts – Nuclide_wnd-counts
  - Does Nuclide_wnd-counts have Poisson distribution? – NO
  - Therefore the requirements are not met -> we should not use Currie!

  - Because the ISO 11929 has no special requirements, we can try to use it
  - Is it possible to determine MDA for WND by using ISO 11929? – YES
  - Is it easy to determine MDA for WND by using ISO 11929? – NO
  - ISO 11929 leads to very complicated formulas describing variation of the resulting activities -> the value of MDA has to be calculated numerically by using appropriate solvers (SW)

Comparison of ISO 11929 and Currie MDA for Extended WND method



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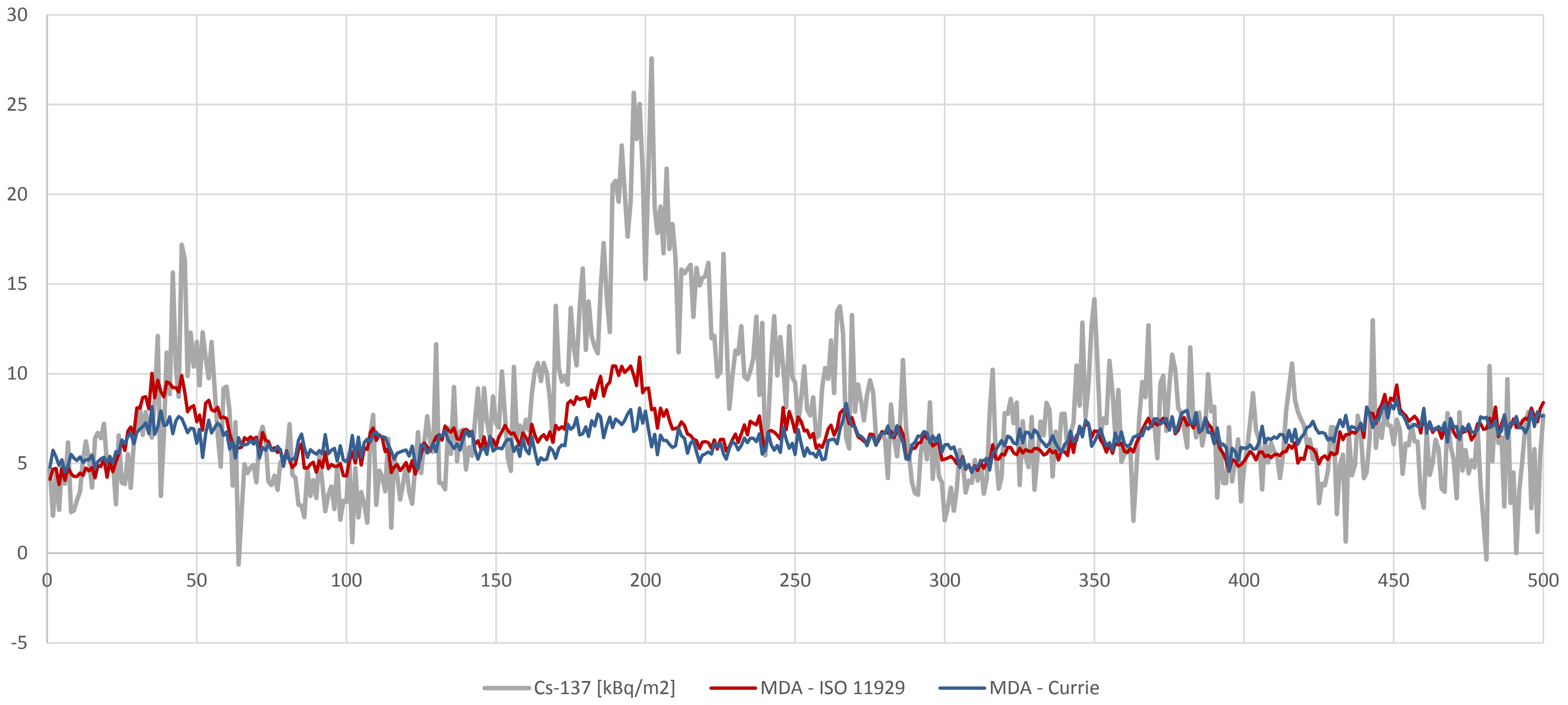

Comparison of ISO 11929 and Currie MDA for Extended WND method

Conclusion

- Currie MDA does not precisely correspond to true variation of resulting values
- However, Currie is simple to calculate and for some cases give us similar results as ISO MDA -> but it should not be reason why to use it!

- ISO MDA precisely corresponds to true variation of resulting values
- ISO MDA can include uncertainty of various inputs (altitude, efficiencies, …)
- ISO MDA is not simple to calculate manually, but it is already implemented in AGAMA SW
- It would be interesting to perform experimental verification of MDA for airborne gamma-ray spectrometry

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