A Monte Carlo Method for uncertainty calculation in gamma spectrometry

Henrik Ramebäck, Petter Lindgren
Swedish Defence Research Agency, FOI

Gammaray 2018, Reykjavik

FOI

Outline

- Why Monte Carlo methods?
- The principle of MCM
- Data sampling
- MC calculations using Excel
- Data analysis
- Examples: activity measurements for two different PDF of a correction factor k_{ET}
- Consequenses on decisions

Monte Carlo Methods (MCM)

- Provides a better estimate of the uncertainty when:
  -There are non-linearities and the uncertainties are not small enough (*higher-order terms can be used in uncertainty propagation, but it might be 'exhausting', and it will not always solve the problem if uncertainties still are too large*)

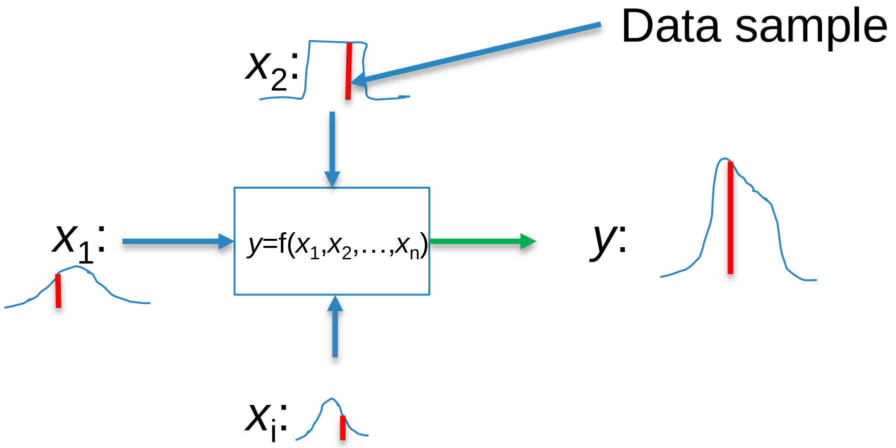
$$u_c^2(y) = \sum_{i=1}^{N}\left(\frac{\partial f}{\partial x_i}\right)^2 u^2(x_i) + \sum_{i=1}^{N}\sum_{j=1}^{N}\left(\frac{1}{2}\left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)^2 + \frac{\partial f}{\partial x_i}\frac{\partial^3 f}{\partial x_i \partial x_j^2}\right)u^2(x_i)u^2(x_j)$$

  -There are non-Gaussian distributed input quantities which contributes significantly to the combined uncertainty
  (PDF known and non-Gaussian, or from assumptions)
- Provides a better estimate of the probability density function (PDF) of the measurand (based on the assumptions of the PDF of the input quantities)
  -*Uncertainty propagation: Gaussian distributions assumed for the measurand*

FOI

MC calculation: Principle

Propagation of distributions:



Data is sampled randomly from the PDFs of each input quantity
➔Many data needed to ensure sampling from the tails of e.g. Gaussian PDF

Calculation tools

- MATLAB
- Other programming language(s)
- Here: Excel
- Advantages using Excel:
  -Widely available
  -No knowledge in programming required
- Disadvantage:
  -Might be somewhat slow(er)…

Excel for MC calculations

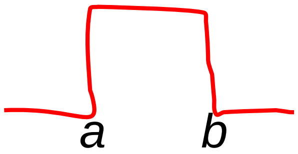
- Pseudo random number generation required for data sampling
- Excel:
  RAND() gives pseudo random numbers between 0-1 (rectangular distributed)
- Early Excel versions (<2010) were considered unreliable in calculating random numbers
- Later versions (>2010) has shown to be fit-for-purpose
  (A. Kallner, Clinica Chimica Acta, 438, 210, 2015)

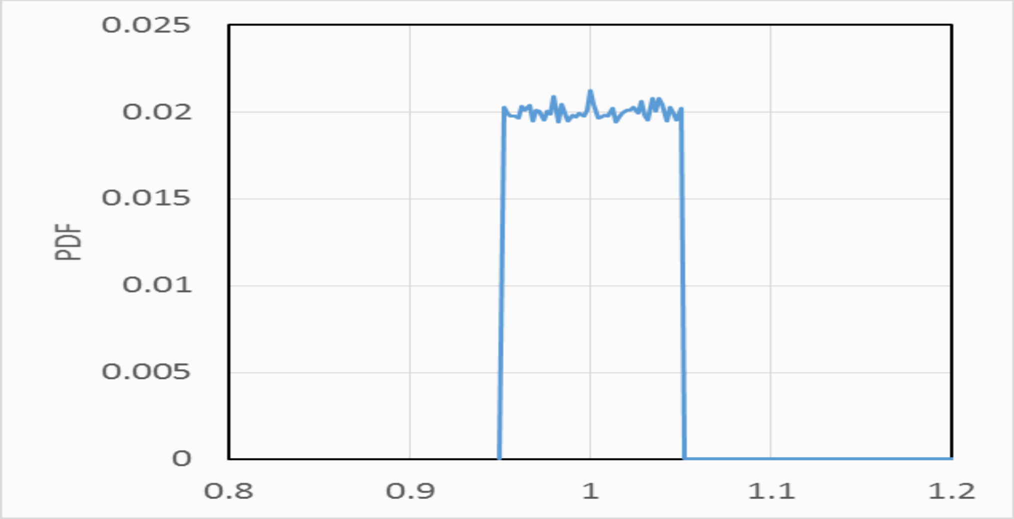
FOI

Data sampling: Rectangular distribution

Rectangular distribution:

- Random samples from the distribution:
- $x = a + (b - a) \cdot \mathrm{RAND}()$
- m=100 000:



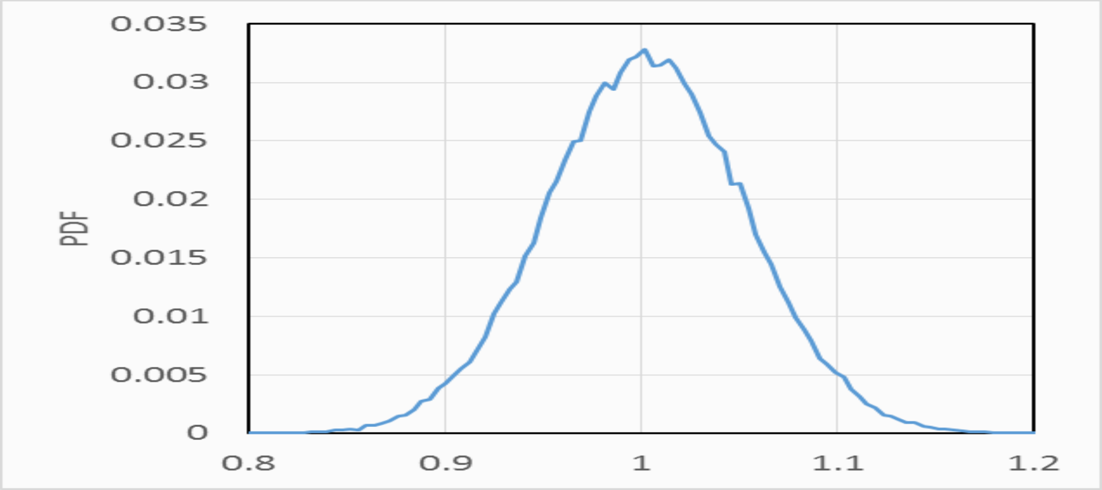


Data sampling: Normal distribution

Normal distribution:

- Random samples from the distribution :

- *x*=NORM.INV(*prob; mean; std unc*)
  prob=RAND()
- *m*=100 000:



Data analysis

- Analyse the measurand with respect to mean, standard deviation and confidence interval (CI):
  -AVERAGE(*range*)
  -STDEV(*range*)
  CI:
  -PERCENTILE(*range*; *prob.*) gives CL for a given *probability*
  Ex: For 95% CI calculate
  -PERCENTILE(*range*; 0.025) and PERCENTILE(*range*; 0.975)

Calculation time

Calculation time in Excel:

- A model equation for gamma spectrometry

  $A = N/(Eff \cdot k_{ET} \cdot I_g \cdot t)$
  $Eff = N_{cal}/(t_{cal} \cdot I_g \cdot A_{cal})$

  and the generation of 600 000 random samples (6·100 000):
  <1 s to calculate mean, standard deviation and the CI
- With the calculation of the PDF it takes about 4 s… (*might be done in a better way…*)
  ➔Good idea to set Excel to manual calculation when a PDF is calculated!

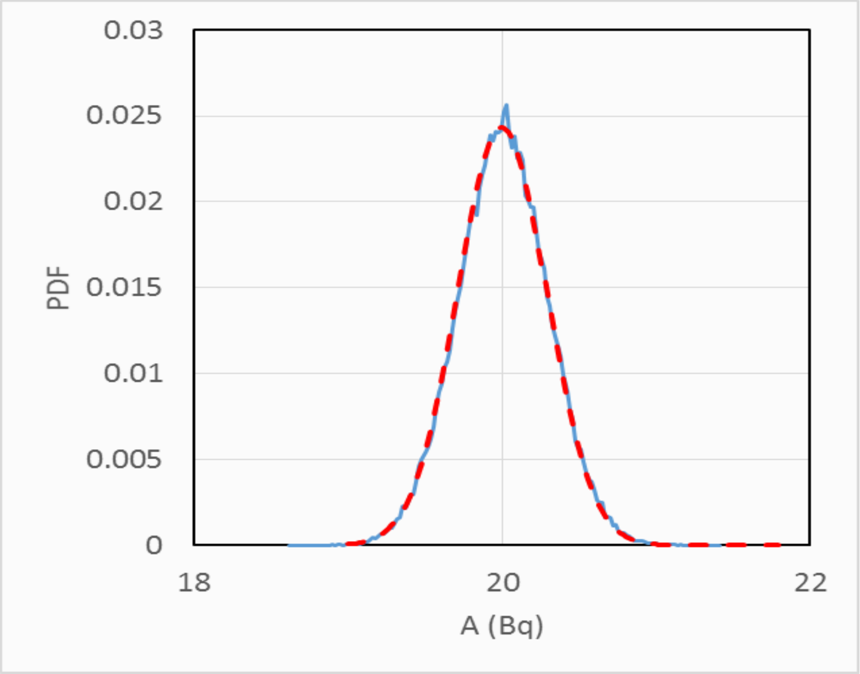
Validation

- The MC calculation in Excel was validated using GUM Workbench Pro 2.4
- GUM Workbench Pro 2.4 calculates uncertainties using uncertainty propagation, but can also run a MC calculation for the same model
- *For equal no. of data samples, Excel and GUM Workbench were consistent with respect to the calculated average, standard uncertianty and CI*

Examples: Efficiency transfer

- $A = N/(Eff \cdot k_{ET} \cdot I_g \cdot t)$
  $Eff = N_{cal}/(t_{cal} \cdot I_g \cdot A_{cal})$
- Case 1:
  Uncertainties, norm.dist., k=1:
  -N: 1%
  -I_g: 0.1%
  -t and t_{cal} set to constants…
  -N_{cal}: 0.3%
  -A_{cal}: 1%
  -k_{ET}: 0.1% (~ref. geo.)

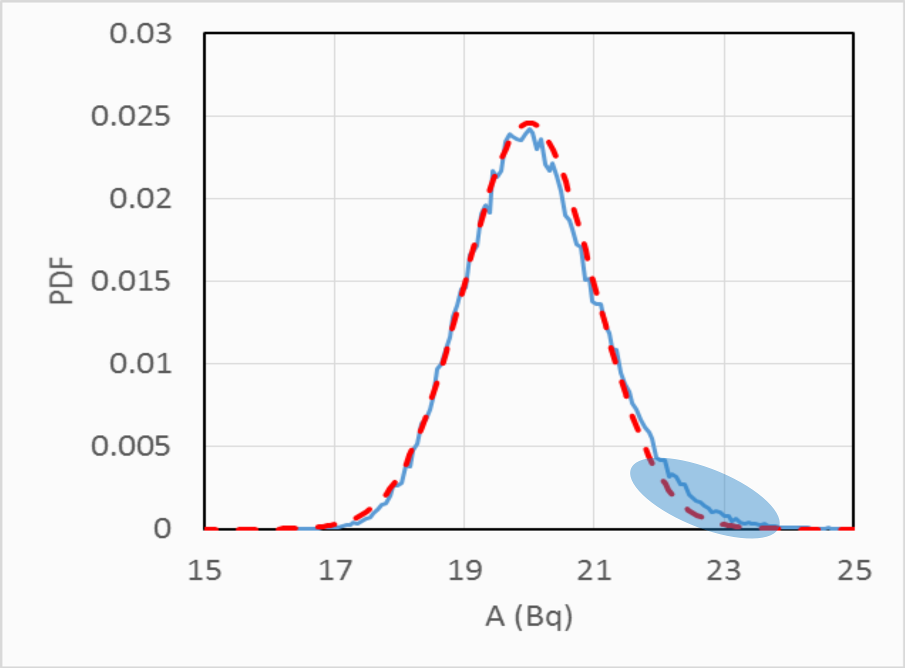
  -Small unc➔No difference!



Dashed red: Uncertainty propagation

Examples: Efficiency transfer

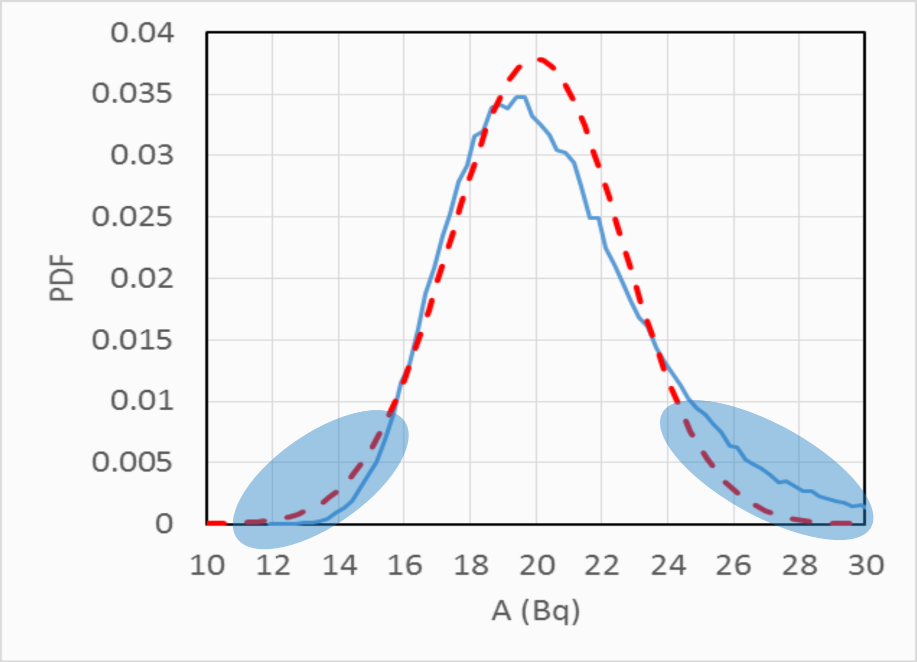
- $A=N/(Eff \cdot k_{ET} \cdot I_g \cdot t)$
  $Eff=N_{cal}/(t_{cal} \cdot I_g \cdot A_{cal})$
- Case 2:
  Uncertainties, norm.dist., k=1:
  -N: 1%
  -I_g: 0.1%
  -t and t_{cal} set to constants…
  -N_{cal}: 0.3%
  -A_{cal}: 1%
  -k_{ET}: 5%



Dashed red: Uncertainty propagation

Examples: Efficiency transfer

- $A = N/(Eff \cdot k_{ET} \cdot I_g \cdot t)$
  $Eff = N_{cal}/(t_{cal} \cdot I_g \cdot A_{cal})$
- Case 3:
  Uncertainties, norm.dist., k=1:
  -N: 1%
  -I_g: 0.1%
  -t and t_{cal} set to constants…
  -N_{cal}: 0.3%
  -A_{cal}: 1%
  -k_{ET}: 15%



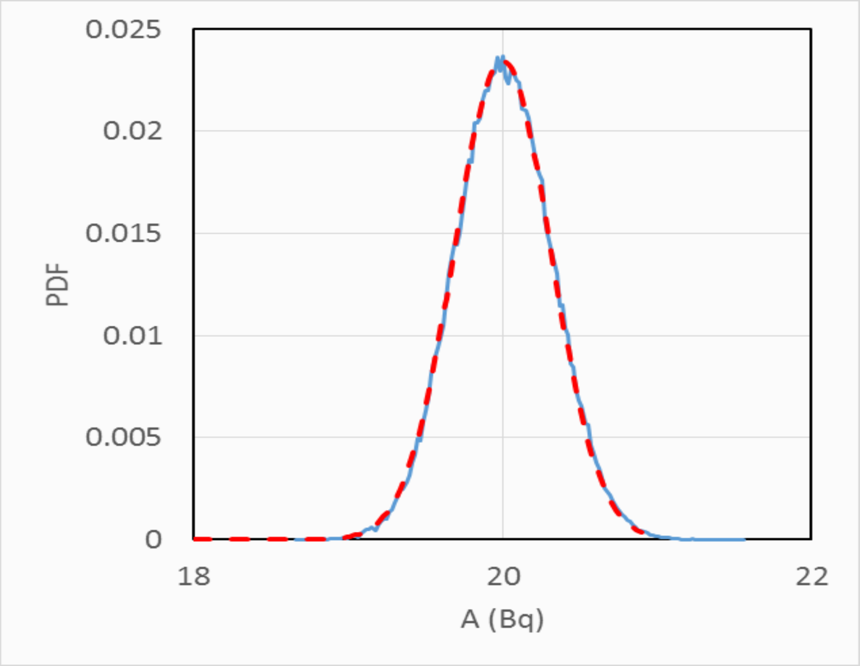
Dashed red: Uncertainty propagation

FOI

Examples: Efficiency transfer

- $A=N/(Eff \cdot k_{ET} \cdot I_g \cdot t)$
  $Eff=N_{cal}/(t_{cal} \cdot I_g \cdot A_{cal})$
- Case 4:
  Uncertainties (rect. dist.):
  -N: 1%
  -I_g: 0.1%
  -t and t_{cal} set to constants
  -N_{cal}: 0.3%
  -A_{cal}: 1%
  -k_{ET}: 1% rect. dist. (half-width)

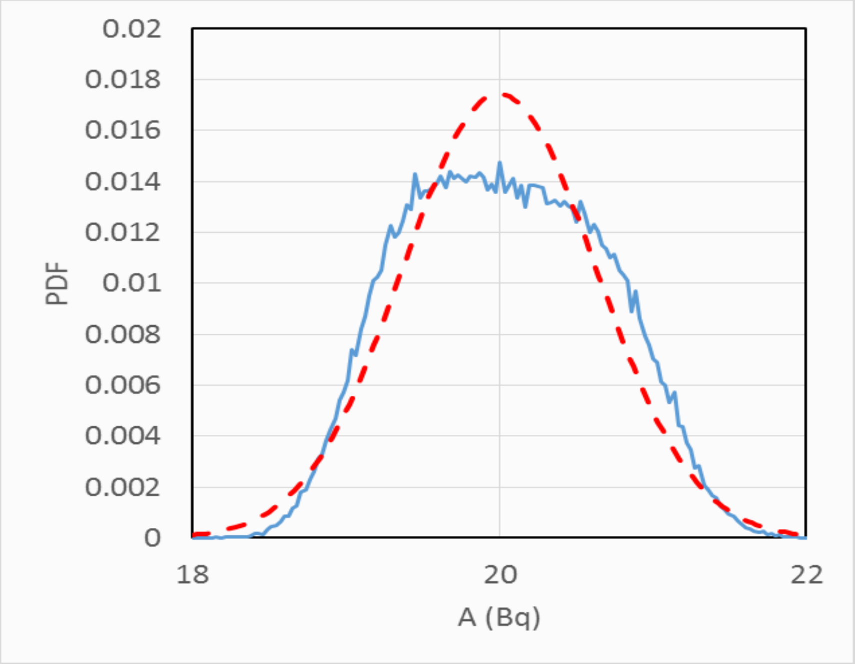
Small unc → No difference!



Dashed red: Uncertainty propagation

Examples: Efficiency transfer

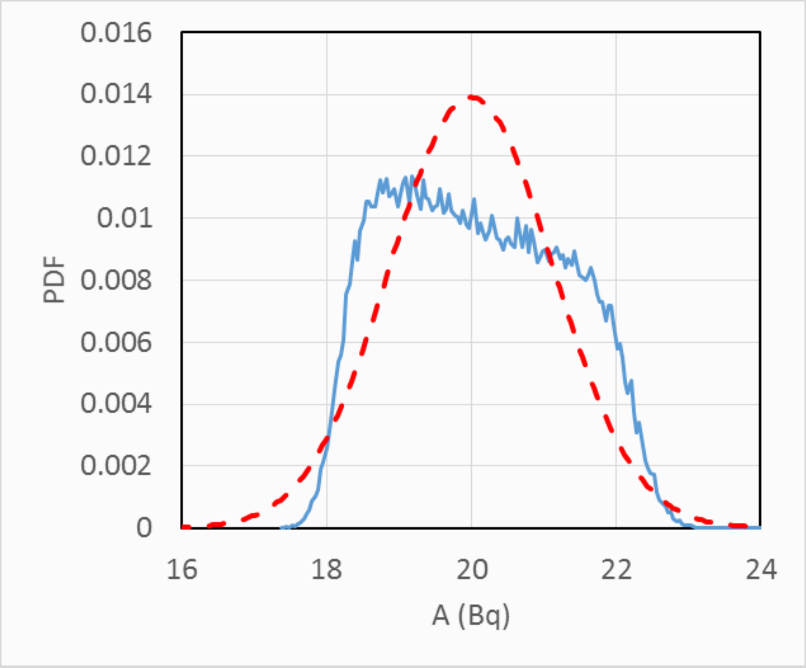
- $A = N/(Eff \cdot k_{ET} \cdot I_g \cdot t)$
  $Eff = N_{cal}/(t_{cal} \cdot I_g \cdot A_{cal})$
- Case 5:
  Uncertainties (rect. dist.):
  -N: 1%
  -I_g: 0.1%
  -t and t_{cal} set to constants
  -N_{cal}: 0.3%
  -A_{cal}: 1%
  -k_{ET}: 5% rect. dist. (half-width)



Dashed red: Uncertainty propagation

Examples: Efficiency transfer

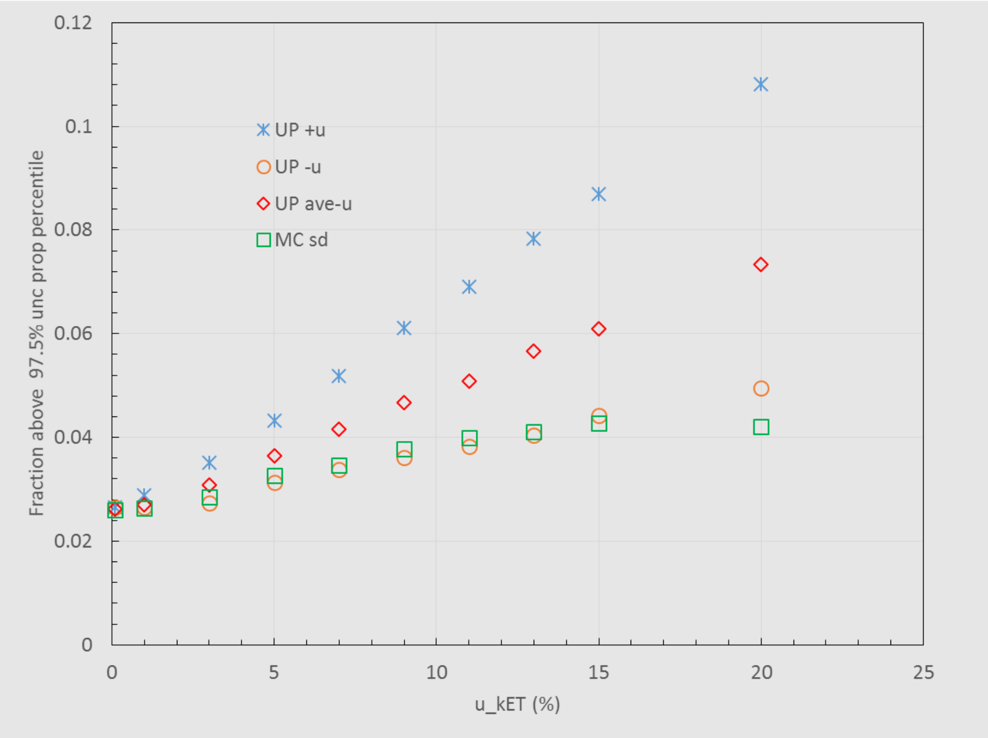
- $A=N/(Eff \cdot k_{ET} \cdot I_g \cdot t)$
  $Eff=N_{cal}/(t_{cal} \cdot I_g \cdot A_{cal})$
- Case 6:
  Uncertainties (rect. dist.):
  -N: 1%
  -I_g: 0.1%
  -t and t_{cal} set to constants
  -N_{cal}: 0.3%
  -A_{cal}: 1%
  -k_{ET}: 10% rect. dist. (half-width)



Dashed red: Uncertainty propagation

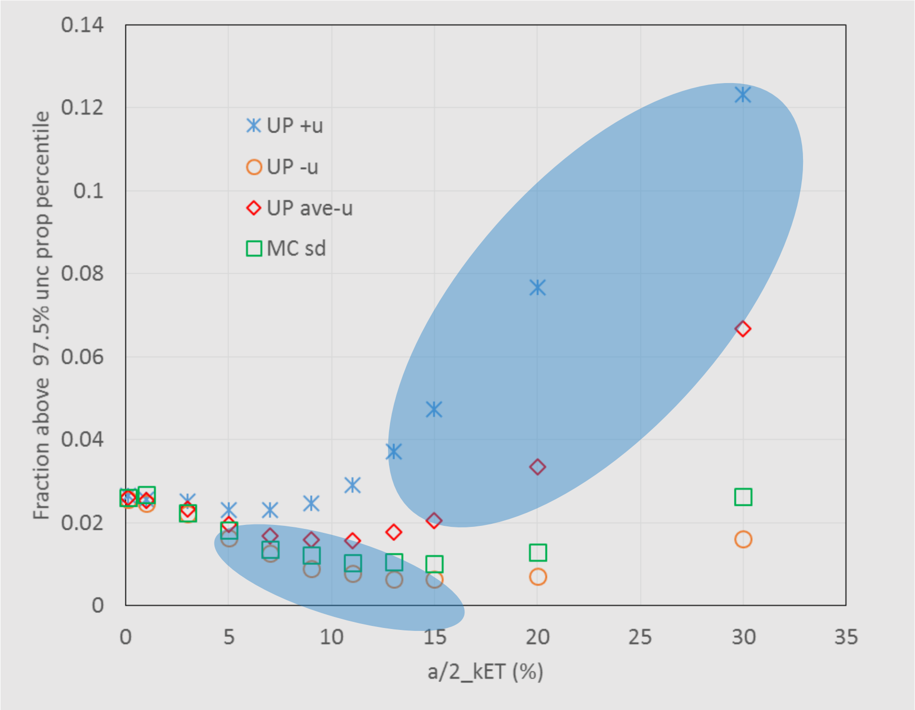
Consequences: k_{ET} normal distribution

Increased risk due to an underestimation of the uncertainties using uncertainty propagation!



Consequences: k_{ET} rectangular distribution

Initially an increased cost using uncertainty propagation (overestimation)…later an increased risk (underestimation)



A general reference to MCM for uncertainty calculations

- *Evaluation of measurement data – Supplement 1 to the "Guide to the expression of uncertainty in measurement" – Propagation of distributions using a Monte Carlo method*, JCGM 101:2008

FOI

Summary

- Excel was used for MC calculation of measurement uncertainty
- Excel showed to be *fit-for-purpose* for MC calculations of the measurement uncertainties in gamma spectrometry, and resulted in consistent results compared to MCM using GUM Workbench Pro 2.4
- The analyst should be aware of the limitations of uncertainty propagation when ’large’ uncertainties of non-linear input quantities exist
- Of course, this also applies to other measurements we might do and when non-linearities exists…

FOI