The Increasing Role of Computer Models in Nuclear Material Assay

Concepts/Outline:

Computer model uncertainty is large component of uncertainty in many situations

This talk focuses on the MCNP code in the context of SNM assay

In the SNM assays of interest, the count rates (CRs) of gamma and neutron radiation depend on the SNM mass but ALSO ON physical properties of the item.

MCNP's role: adjust the CRs for these physical properties in order to estimate SNM mass

Example 1: Shuffler

Example 2: Distributed Source Term Analysis of holdup

Both Examples: MCNP errors result in "errors in predictors"

Tom Burr, Statistics Group
David Beddingfield, Stephen Tobin, Safeguards Science and Technology Group
Los Alamos National Laboratory

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1. What does a Shuffler do?

Determines the *mass of fissile isotopes* (^{235}U, ^{239}Pu, etc., which are SNM) by detecting *delayed-neutrons* from fission fragments that were produced by induced fissions.

The neutrons inducing fissions were produced by the spontaneous fission of *^{252}Cf*.

The delayed-neutrons are emitted from *daughter products* that were produced by *induced fissions*.

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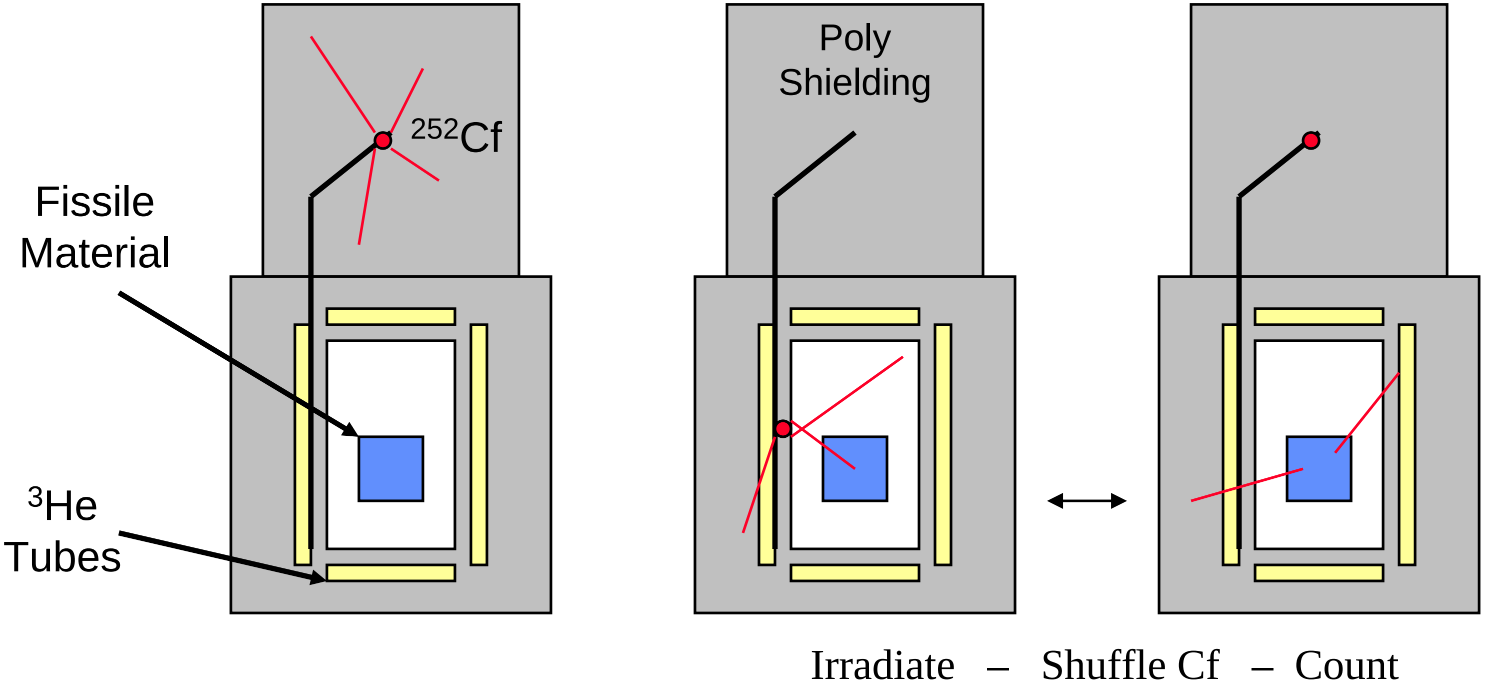
Schematic of Shuffler Operation



- Irradiate with neutrons from ^{252}Cf, remove ^{252}Cf, then count delayed-neutrons.
- "Shuffle" the ^{252}Cf in and out of the assay chamber to reach the desired precision.

“Standard” 55-gallon Drum Shuffler

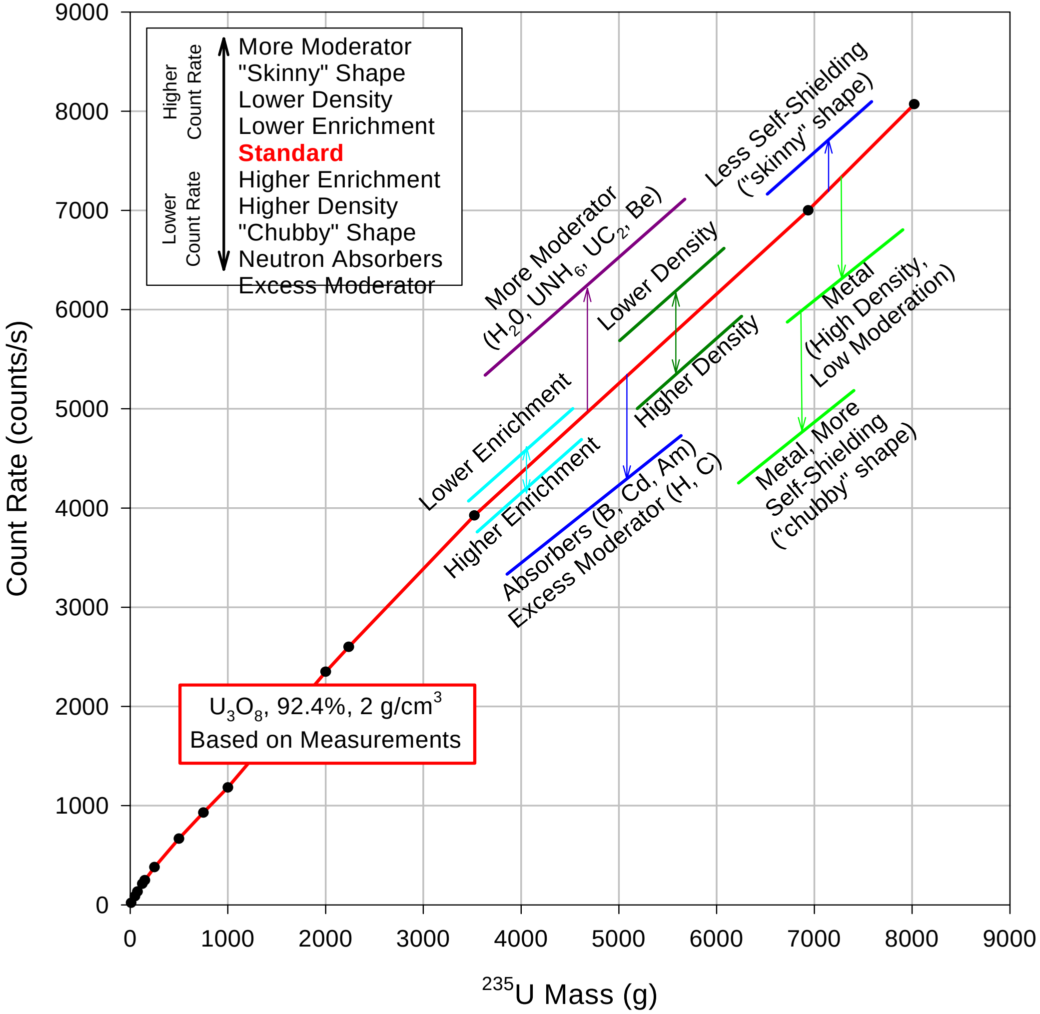
Performs active neutron assays for ^{235}U routinely in 16 minutes.

Without significant error, the delayed-neutron precursors can be organized into *6 groups*. Each group has *one half-life* and produces an *average number of delayed-neutrons per initial fission*

A detailed *theoretical understanding of the fundamental physics allows quantitative calculations* of shuffler count rates, including the impact of effects such as sample properties, shape, density chemical form (metal, oxide, liquid or gas), enrichment, etc.

This LANL-designed shuffler is available from Canberra.

Traditional Calibration Curve with Qualitative Biases Included



- *Traditional calibration* -indicated by red line for U_30_8, 92.4% ^{235}U and 2 g/cm^3 –*count rate vs. mass determined from multiple standards*.
- *Biases* represent difference between standards used for calibration and the unknown.
- For a traditional calibration, biases are minimized by *making unknown and sample as alike as possible*.
- Thus, sample properties, shape, density, chemical form (metal, oxide, liquid or gas), enrichment, etc. must be matched. Clearly, this can not be done for all cases.

Calibration/Estimation

Calibration:

CR = M *x* F1 *x* F2 *x* F3 + error   during calibration with standards

F1is the expected total number of counts (over all cycles) per source ^{252}Cf neutron per gram of SNM **via MCNP**

F2 is a constant (ratio of irradiation time to count time)

F3 is the least squares estimate that has an interpretation as the pseudo ^{252}Cf neutron source strength (^{252}Cf neutron generator is not modeled by MCNP)

Estimation:

M = CR/(F1 *x* F2 *x* F3) + error

There is no interest in F1, F2, or F3. The goal is to estimate M. Therefore, "errors in predictors" literature is of limited value: if calibrate using "corrupted" predictor F1 then corrupted F1 is adequate in future assays.

Issues regarding Uncertainty Quantification (UQ)

1. Measurement categories

Unmodeled effects impact new measurement categories in unknown ways. Examples: hold in Cd liner on detector bank is not modeled; air gap in polyethylene blocks is not modeled, others.

Perturb inputs to MCNP. **Assume** MCNP models all relevant effects for given measurement category.

“Costly approach:” remeasurement of some items using alternate method (calorimetry)

Typically: need to partition total error variance into: Random, “systematic” so estimate confidence limits for items and for sums of items.

Example: $\text{Meas} = T + S_{\text{category}} + S_{\text{item}} + R$

2. Suggest use cross validation in “estimate pseudo-source-strength” calibration step.

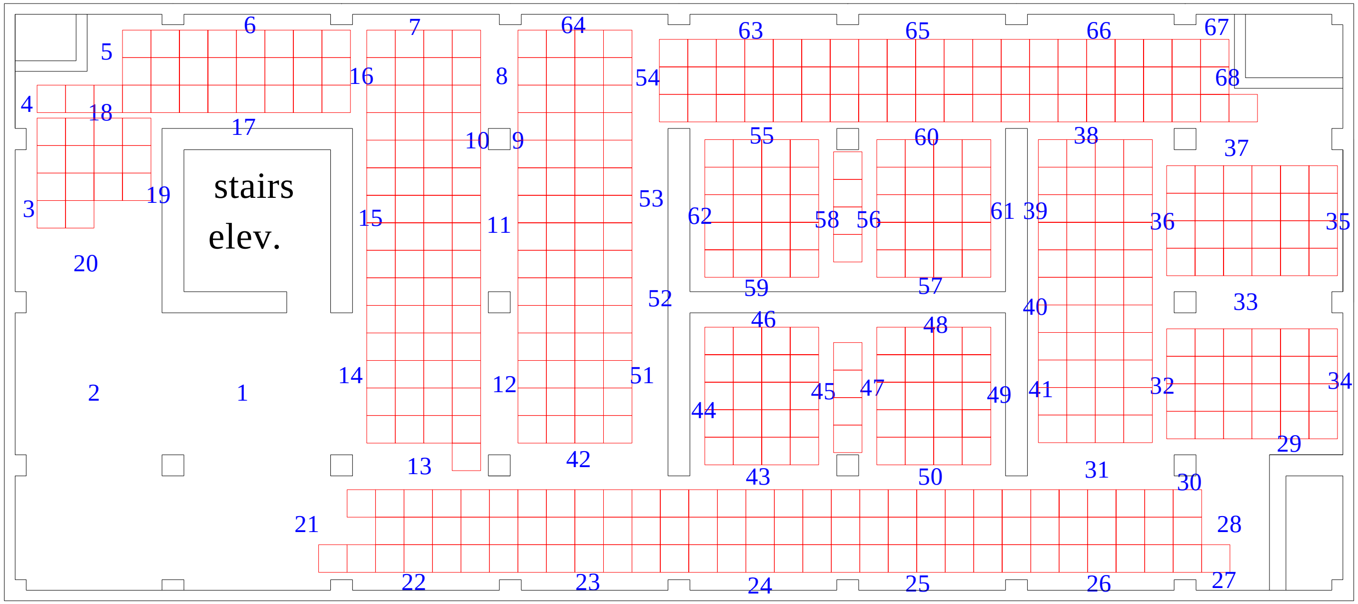
2. Distributed Source Term Analysis of Holdup

Source locations inside red rectangles

Neutron measurement positions (detector locations) numbered in blue

Goal: Estimate total source using MCNP-corrected neutron count rates.

Use ½ of the measurement positions to produce estimate 1, other ½ to produce estimate 2. Compare estimates.



SNM estimation and error analysis

$$M_p \sim \text{Poisson}\left(t \sum_V R_{VP} A_V\right) \Big/ t$$

$E(MP)$ = the expected measured count rate at position P [counts/second]
A_V = the source activity in voxel V [neutrons/second]
R_{VP} = the $V \times P$ detector response matrix from neutrons produced in voxel V for the detector in position P [counts/neutron]

GOAL: Estimate $\sum_V A_V$

Error analysis: (1) ignore errors in R_{VP}; *(2)* consider errors in R_{VP}

Regarding errors in R_{VP}:

MCNP “tallies” include notion of random error.

^{252}*Cf source neutron detected count rates vs predicted addresses “systematic error”*

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Issues

Constraint: true neutron source strengths in each voxel $A_V \geq 0$

Error variance depends on A_V

Possible? Closed form solution for constrained WLS, with or without attention to errors in predictors (EIP).

EIP: the 0 entries in are "true 0's." Suggests multiplicative model, but need systematic and random error in R_{VP}

Our status: relying on simulation, with and without SIMEX, and with and without nonnegativity constraint.

Prefer faster, closed form approximations, preferably for Excel.

Table 1. Estimate of Neutron Source Strength and RAE ignoring and then including errors in R_{VP} and using 1000 simulations to confirm the theoretical RAE result.
The RAE results in Column 6 for rows 7, 8, and 9 did not use SIMEX.

RAE (Theoretical and confirmed by Simulation) This ignores error in R_{VP} . (Case 1)	Condition of R_{VP} ($d_{\max}/d_{\min}$)	RAE SIMEX* simulation results. This includes error in R_{VP} . (Case 2)
A: 1% B: 1%	A: 40.3 B: 34.2	A: 24% B: 26%
A: 0.6%, B: 0.6%	A: 34.7 B: 35.9	A: 12% B: 7%
A: 2% B: 2%	A: 13.4 B: 13.0	A: 7% B: 5%
A: 8% B: 10%	A: 36.8 B: 35.3	A: 17% B: 13%
A: 6% B: 8%	A: 15.6 B: 20.6	A: 21% B: 27%
A: 3% B: 3%	A: 22.7 B: 22.2	A: 9% B: 10%
Group 1: A: 4% B: 5% Group 2: A: 1% B: 1%	Group1: A: 198.7 B: 229.5 Group2: A: 14.9 B: 20.9	Group 1: A:12% B:12% Group 2: A: 9% B: 9%
A: 48% B: 27%	A: 6741.8 B: 4223.5	A: 6% B: 9%
A: 24% B: 23%	A: 1162.5 B: 1049.0	A: 15% B: 21%

RAE is the relative absolute error

SIMEX performance worse than WLS in some cases

Note: the last 2 rows show better results when include EIP –but rows 7,8,9 used WLS, not SIMEX. If use SIMEX, then RAE >50%

Summary

Need sensitivity study to assess impact of $\hat{A}_V$

Constrained or unconstrained WLS sometimes doing better than SIMEX (rows 7,8,9). In some cases, the price for bias reduction using SIMEX is large variance increase.

Relying on simulation. Can we get analytical approximations.

If have to rely on simulation, might as well try “fully Bayes.”