Uncertainty propagation

- TREAT single standard fuel assembly
- SERPENT
- Fuel composition, uranium isotopes, geometry parameters studied
- Parameter values chosen based on the BATMAN report
- Goal: compare methods and understand the details to prepare for a full core study

Issues in previous uncertainty propagation results

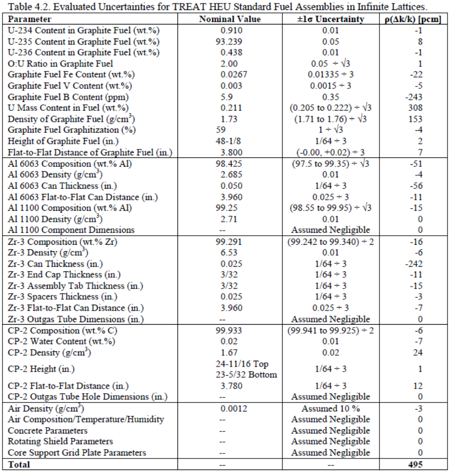

Table 4.2. Evaluated Uncertainties for TREAT HEU Standard Fuel Assemblies in Infinite Lattices.

Parameter	**Nominal Value**	**±1σ Uncertainty**	**ρ(Δk/k) [pcm]**
U-234 Content in Graphite Fuel (wt.%)	0.910	0.01	-1
U-235 Content in Graphite Fuel (wt.%)	93.239	0.05	8
U-236 Content in Graphite Fuel (wt.%)	0.438	0.01	-1
O:U Ratio in Graphite Fuel	2.00	0.05 ÷ √3	1
Graphite Fuel Fe Content (wt.%)	0.0267	0.01335 ÷ 3	-22
Graphite Fuel V Content (wt.%)	0.003	0.0015 ÷ 3	-5
Graphite Fuel B Content (ppm)	5.9	0.35	-243
U Mass Content in Fuel (wt.%)	0.211	(0.205 to 0.222) ÷ √3	308
Density of Graphite Fuel (g/cm^3)	1.73	(1.71 to 1.76) ÷ √3	153
Graphite Fuel Graphitization (%)	59	1 ÷ √3	-4
Height of Graphite Fuel (in.)	48-1/8	1/64 ÷ 3	2
Flat-to-Flat Distance of Graphite Fuel (in.)	3.800	(-0.00, +0.02) ÷ 3	7
Al 6063 Composition (wt.% Al)	98.425	(97.5 to 99.35) ÷ √3	-51
Al 6063 Density (g/cm^3)	2.685	0.01	-4
Al 6063 Can Thickness (in.)	0.050	1/64 ÷ 3	-56
Al 6063 Flat-to-Flat Can Distance (in.)	3.960	0.025 ÷ 3	-11
Al 1100 Composition (wt.% Al)	99.25	(98.55 to 99.95) ÷ √3	-15
Al 1100 Density (g/cm^3)	2.71	0.01	0
Al 1100 Component Dimensions	--	Assumed Negligible	0
Zr-3 Composition (wt.% Zr)	99.291	(99.242 to 99.340) ÷ 2	-16
Zr-3 Density (g/cm^3)	6.53	0.01	-6
Zr-3 Can Thickness (in.)	0.025	1/64 ÷ 3	-242
Zr-3 End Cap Thickness (in.)	3/32	1/64 ÷ 3	-11
Zr-3 Assembly Tab Thickness (in.)	3/32	1/64 ÷ 3	-15
Zr-3 Spacers Thickness (in.)	0.025	1/64 ÷ 3	-3
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Zr-3 Outgas Tube Dimensions (in.)	--	Assumed Negligible	0
CP-2 Composition (wt.% C)	99.933	(99.941 to 99.925) ÷ 2	-6
CP-2 Water Content (wt.%)	0.02	0.01	-7
CP-2 Density (g/cm^3)	1.67	0.02	24
CP-2 Height (in.)	24-11/16 Top 23-5/32 Bottom	1/64 ÷ 3	1
CP-2 Flat-to-Flat Distance (in.)	3.780	1/64 ÷ 3	12
CP-2 Outgas Tube Hole Dimensions (in.)	--	Assumed Negligible	0
Air Density (g/cm^3)	0.0012	Assumed 10 %	-3
Air Composition/Temperature/Humidity	--	Assumed Negligible	0
Concrete Parameters	--	Assumed Negligible	0
Rotating Shield Parameters	--	Assumed Negligible	0
Core Support Grid Plate Parameters	--	Assumed Negligible	0
Total	--	--	**495**

Baseline assessment of TREAT for modeling and analysis needs (batman report), table4.2)

- Boron impurity uncertainty
- No correlation between variables
- No "covariance data" available between parameters

Methodology

Parameter choices and separation

- Group1-Uranium vector: $U234,\ U235,\ U236,\ U238$
- Group2-Fuel composition: $B,\ O,\ U,\ C,\ V,\ Fe$ (V, Fe wt% and O:U ratio were kept as constants in samples⇒ three variables)
- Group3-Al 6063 composition
- Group4-Al can thickness
- Group5-Zr can thickness

Uncertainty propagation

- Method 1: Sandwich rule
- Method 2: Stochastic sampling

Build covariance matrix

- Covariance matrices built for the first two group
- Uranium vector constraint function:
  $$U234wt\% + U235wt\% + U236wt\% + U238wt\% = 100\%$$
- Fuel composition constraint function:
  $$\frac{31.98983}{235.1999} \cdot Uwt\% + 0.0267 + 0.003 + \frac{Bppm}{10000} + Uwt\% + Cwt\% = 100$$
- Each parameter is expanded at its nominal value in terms of partial derivatives of with respect to the other parameters

$$\begin{aligned} cov(x_1, x_2) &= E[(x_1 - \bar{x_1})(x_2 - \bar{x_2})] \\ &\approx E[(\sum_{i \neq 1} \frac{\partial x_1}{\partial x_i}|_{\vec{\bar{x}}}(x_i - \bar{x_i}))(\sum_{i \neq 2} \frac{\partial x_2}{\partial x_i}|_{\vec{\bar{x}}}(x_i - \bar{x_i}))] \end{aligned}$$

$\frac{\partial x_i}{\partial x_j}|_{\vec{\bar{x}}}$ is evaluated using the constraint function

Covariance matrices

- Uranium vector: (U234, U235, U236, U238)(wt%)

$$\begin{pmatrix} 6.400\text{E-}5 & 5.683\text{E-}5 & 8.205\text{E-}7 & -5.272\text{E-}6 \\ & 6.760\text{E-}4 & -5.830\text{E-}5 & -2.218\text{E-}4 \\ & & 6.400\text{E-}5 & -4.334\text{E-}6 \\ & & & 2.560\text{E-}4 \end{pmatrix}$$

- Fuel composition: (Bppm, Uwt%, Cwt%, Owt%)

$$\begin{pmatrix} 1.350 & -1.648\text{E-}6 & -1.331\text{E-}4 & -2.242\text{E-}7 \\ & 1.600\text{E-}5 & -1.808\text{E-}5 & 2.166\text{E-}7 \\ & & 2.500\text{E-}5 & -2.460\text{E-}6 \\ & & & -2.946\text{E-}7 \end{pmatrix}$$

Sensitivity coefficients

- $\frac{\alpha}{k}\frac{k}{\partial\alpha}$: percent change of k_{eff} caused by percent change of the input α
- Effect on k_{eff} caused by one parameter has two parts: explicit sensitivity and implicit sensitivity, $S_{complete} = S_{implicit} + S_{explicit}$
- For uncertainty propagation purpose, the sensitivity coefficients used in sandwich rule should be $S_{explicit}$ (implicit part is considered in the covariance matrix)
- Multiple linear regression. Regression model:

$$a_1x_1 + a_2x_2 + \cdots + a_nx_n = k_{eff}$$

- No intercept term in the model (consideration from the multicollinearity point of view, which will be discussed later)

Sample generation

- Strong correlation between parameters (composition and geometry parameters)
- Perfect Multicollinearity: a set of n random variables which satisfy:

$$a_0 + a_1x_1 + a_2x_2 + \cdots + a_nx_n = 0$$

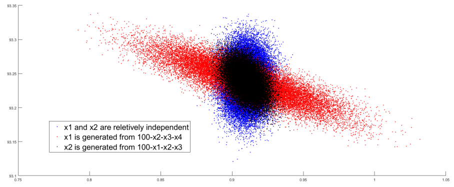
- It's called "perfect" but you want to avoid it. Usually it means data redundant during the "translation" of a physical model into math

$$\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \begin{pmatrix} & \cdots & \\ \vdots & & \\ & \textit{response matrix} & \\ & & \end{pmatrix} \rightarrow \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix}$$

To avoid multicollinearity

Method 1: parameter reduction

Keep one parameter unchanged/as a balance parameter.



Method 2: Consider all parameters

First generate sample for each variable independently, then normalize the varables by the constraint function

Sample generation: example of group2 (fuel composition)

- wt%s of Fe and V and O:U ratio are kept as constants. (V wt%=0.003, Fe wt%=0.0267, O:U=2)
- Define four dummy variables: $x_1,\ x_2,\ x_3$

$$x1 \sim \mathcal{N}(\mu = 7.53ppm,\ \sigma = 1.16ppm)$$

$$x2 \sim \log(\mathcal{N})(\mu = -1.5561,\ \sigma = 0.018956)$$

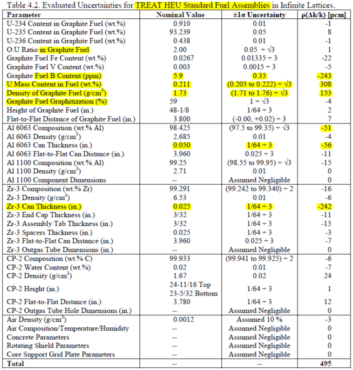
$$\leftarrow \textit{best fits the measured data range of uranium}$$

$$x_3 \sim \mathcal{N}(\mu = 99.7298wt\%,\ \sigma = 0.005)$$

- Define normal factor as
$$N = \frac{100}{\frac{31.98983(Atomic\ \ mass\ \ of\ \ O\times 2)}{235.1999}x_2 + 0.0267 + 0.003 + \frac{x_1}{10000} + x_2 + x_3}$$
- Variables to use in the input files are calculated as: B (ppm)= Nx_1, U (wt%)= Nx_2, C (wt%)= Nx_3, O (wt%)=$\frac{31.98983}{235.1999}Nx_2$
- Natural isotopic composition and density of the fuel are kept as constants

Sample size

- Samples for different parameter groups are generated independently
- Sample size for each parameter group is determined by its "importance"
- Based on the single assembly results in BATMAN report:



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Parameter group	Stochastic sample size
Uranium vector	50
Fuel composition	150
Al 6063 composition	50
Al can thickness	100
Zr can thickness	100

Other issues/details

- Parameters in Al 6063 composition group:
    - Al component used as a balance factor
    - other element samples generated assuming uniform distributions
    - natural isotopic composition and density of Al6063 kept constants
- Al can thickness and Zr can thickness:
    - assumed independent from any other variables
    - acceptable for single assembly model
    - change when run full core problem
- Both Al can and Zr can inner radius were kept as constants, outer radius were perturbed to give perturbation on thickness

Results

Parameter group	Stochastic sample size	Stochastic results
Uranium vector	50	mean $k_{eff} = 1.4117$, $std = 17.5pcm$, $\frac{std}{mean} = 12.4pcm$
Fuel composition	150	mean $k_{eff} = 1.4108$, $std = 1686.8pcm$, $\frac{std}{mean} = 1195.7pcm$
Al 6063 composition	50	mean $k_{eff} = 1.4119$, $std = 32.5pcm$, $\frac{std}{mean} = 22.9pcm$
Al can thickness*	100	mean $k_{eff} = 1.4137$, $std = 1546.8pcm$, $\frac{std}{mean} = 1094.1pcm$
Zr can thickness*	100	mean $k_{eff} = 1.4133$, $std = 1558.4pcm$, $\frac{std}{mean} = 1102.6pcm$

Fuel composition	Sensitivity coefficients $\frac{\alpha}{k} k_\alpha$	Direct Contribution to $(\frac{\partial k}{k})^{**}$
boron (ppm)	-0.076	-1110.6pcm
U (wt%)	0.485	954.4pcm
C (wt%)	0.864	4.1pcm
O (wt%)	-0.273	-538.6pcm

- *: Al can thickness and Zr can thickness samples are generated following uniform distribution. This leads to the divergence in the final results.
- **:$\frac{\partial k}{k}$ is the direct percent change caused by each parameter.
- We planed to perform sensitivity analysis to uranium vector, however the multiple regression results showed poor linearity. Details on next slide.

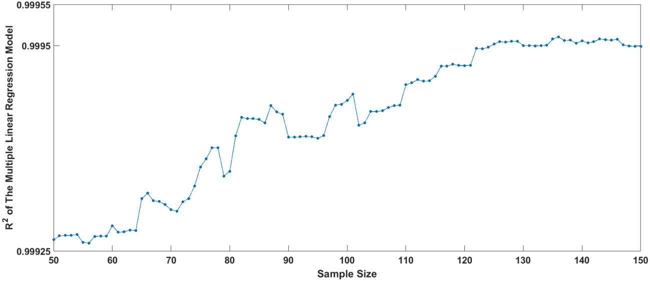
Linearity analysis: running R^2 plots

Uranium vector variables:

- R^2 value much lower than acceptable (~ 0.4)
- Tried increasing sample size to 100, no obvious improvement
- Tried adding higher order terms in the model, improvement not good enough

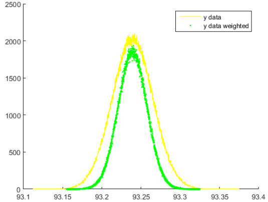
Fuel composition variables:

- High linearity thanks to Boron



Finds and on-going work

- Trying first order perturbation theory to solve for the sensitivity coefficients
- Solving issues with the normalization in sample generation



- Coming up new sample generation ideas to solve the uniform distribution problem
- Try surrogate model