CORRELATION OF HST-001 DUE TO UNCERTAIN TECHNICAL PARAMETERS – COMPARISON OF RESULTS FROM DICE, SAMPLER AND SUnCISTT

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ABSTRACT

In this work we present a detailed uncertainty, correlation and sensitivity study of k_{eff} values with focus on uncertain technical parameters of ten experiments of critical high enriched uranium solutions with a thermal neutron spectrum. The experiments are documented in the ICSBEP as HEU-SOL-THERM-001(HST-001) [1]. The total Monte Carlo approach was chosen to allow all uncertain quantities to be sampled at once following their individual distribution functions. The stochastic dependencies between variables of different experiments were chosen based on available data.

The analyses were done individually and independent by GRS using the code SUnCISTT [2] and ORNL using the SCALE sequence SAMPLER [3]. Both Monte Carlo approaches rely on the neutron transport code KENO from SCALE 6.2.2 [4]. This enables a direct comparison of the implemented total Monte-Carlo methods.

Each of the two codes were used to analyze two different sets of uncertainties: The first evaluation is based on the uncertainties given in chapter 1"Detailed Description" of the HST-001 evaluation in the ICSBEP handbook. The second is based on the evaluated uncertainties given in chapter 2.0 "Evaluation of experimental data".

The uncertainty, sensitivity studies, and Pearson´s correlation coefficients for the k_{eff} values calculated are presented. A comparison with the correlation coefficients given in DICE [5] is discussed.

KEY WORDS

Correlation Coefficient, Critical Experiment, Uncertainty Analysis.

1. INTRODUCTION

By chance, GRS and ORNL performed the same effort to produce covariance and correlation data for the same set of experiments in the scope of the OECD/NEA WPNCS (working party of nuclear criticality safety). These efforts were started completely individually and independent from each other. During the WPNCS meeting in 2018 it was realized that the same set of HST experiments was used based on the same evaluations in the ICSBEP, using the same literature and the same computational approach, but with different actual computational tools. However, some significant differences in the results were found. These differences arouse from different assumptions for the uncertainty data of the benchmark experiments which were both documented in the ICSBEP handbook. A collaboration started with the aim to solve the cause of these differences and to compare the methods of GRS and ORNL to create reliable correlation coefficients.

The motivation for this effort was intensified by comparison with the low fidelity correlation coefficients distributed with DICE. The correlation coefficients in DICE were also not comparable to the received calculational results

For the analysis of all 10 experiments of the experimental series HST-001 a detailed sensitivity, uncertainty and correlation study was performed on uncertain technical parameters. To be able to consider multiple uncertain experimental parameters (e.g. geometric dimensions, enrichment or temperature) at once the total Monte Carlo approach was chosen. Therein all uncertain quantities are sampled at the same time according to their individual distribution functions. The stochastic dependencies between variables of different experiments were chosen carefully according to the given data.

2. DESCRIPTION OF EXPERIMENTS

The experimental series analysed in this paper is taken from the ICSBEP handbook. The experiments were performed in the mid-1970's at Rocky Flats Plant. The series contains ten experiments of critical high enriched solutions of uranyl nitrate with a thermal neutron spectrum, documented as HEU-SOL-THERM-001. The experiments consist of cylinders of different materials (SS-304 or Al-6061) and various diameters (28.01 – 50.69 cm). The aluminium tanks were coated with Phenoline 300 on the inside, which was however neglected in the benchmark model. Criticality was reached by increasing the level of solution in the tank until k_{eff} = 1.0 was reached. Apart to the tank, no further reflection was assumed. This neglects reflections from the room and objects in the room. Further details on the experiments can be found in [1].

3. DESCRIPTION OF CODES AND DATA

The individual criticality calculations were performed with the CSAS5 sequence from the SCALE 6.2.2 code package [4]. Table I and II show the basic details of the calculations by GRS and ORNL.

Table I. Details of the individual criticality calculations of GRS.

Parameter	Value
Code package	SCALE 6.2.2
Sequence	CSAS5
Neutron library	252 energy grouped ENDF/B-VII.1 (v7-252) [6]
Neutrons/generation	10.000
Skipped generations	100
σ_{MC}	1.0 x 10^{-4}
# samples/experiment	250
h_{CPU} / calculation	~ 0.4
$h_{CPU,total}$	~ 4.000

Table II. Details of the individual criticality calculations of ORNL.

Parameter	Value
Codepackage	SCALE 6.2.1
Sequence	CSAS5
Neutron library	238 energy grouped ENDF/B-VII.0 (v7-238)
Neutrons/generation	10.000
Skipped generations	20
σ_{MC}	1.0 x 10^{-4}
# samples/experiment	300
h_{CPU} / calculation	~ 2.5
$h_{CPU,total}$	~ 7500

The methodology used by GRS is based on the GRS tool SUnCISTT (Sensitivities and Uncertainties in Criticality Inventory and Source Term Tool [2]), which controls the uncertainty analysis. It is provided with a template input file of the criticality calculation (e.g. SCALE), a list with randomly generated values of the varied parameters according to the specified distributions, a mapping file assigning values in the list to keywords in the template file and a calculation module for modification of the varied parameters (e.g. diameter to radius). SUnCISTT then generates the executable input files, starts the individual calculations, checks for missing output files, performs the uncertainty analysis for each experiment and determines correlations and covariances between experiments.

ORNL employs the SCALE internal sequence SAMPLER, which also uses the total Monte Carlo approach. Sampler [Section 6.7 of [4]] is referred to as a "super-sequence" within SCALE because it wraps around other sequences, such as CSAS, and perturbs inputs via Monte Carlo sampling. It should be noted that none of the nuclear data sampling capabilities within Sampler are used in the determination of these correlations. The composition and dimension sampling used here is activated with the *perturb_geometry* option.

250 Monte-Carlo samples have been generated and analyzed to ensure converged correlation coefficients. That is a conservative number of samples. Most of the results were already converged after 100 samples. For a detailed description of the convergence of correlation coefficients calculated via Monte-Carlo methods see e.g. [7].

For the sensitivity, uncertainty and correlation study two different sets of uncertainties were used by each of the two institutes: The first evaluation is based on the uncertainties given in chapter 1 "Detailed Description" of the ICSBEP handbook. The second is based on the evaluated uncertainties given in chapter 2.0 "Evaluation of experimental data" of the ICSBEP handbook, especially tables 10.1 to 10.10 of chapter 2.6.

Table III. shows an overview of the uncertain technical parameters and the assumptions made. Since 4 different tanks were used, also 4 sets of outer solution radius (or inner tank radius), tank sidewall thickness and tank bottom wall thickness exist. These technical parameters are correlated between experiments with the same tank. The critical solution height is assumed to be uncorrelated between the experiments, the enrichment correlated between all experiments. Two sets of two experiments each exist which have the same U-density, nitride acid density and total density: experiments 001 and 008, and experiments 004 and 009. Table IV shows the values and experimental uncertainties of the tank parameters for both sets of uncertainties. Table V shows the values and experimental uncertainties of the solution parameters for both sets of uncertainties.

Table III. Overview of the uncertain technical parameters and assumptions made.

Parameter	Shortcut	Value	Uncertainty	Corr
Outer solution radius	solRadOut	4 sets	4 sets	4 sets
Tank sidewall thickness	tankWallThick	4 sets	4 sets	4 sets
Tank bottom wall thickness	tankBottomThick	2 sets	2 sets	4 sets
Critical height of solution	solCritHeight	Individual	Individual	-
Wt% 234U	wt%234U	1.022	0.043	1 set
Wt% 235U	wt%236U	0.434	0.005	1 set
Wt% 236U	wt%238U	5.36	0.036	1 set
U density in solution	solRhoU	8 sets	8 sets	8 sets
Nitride acid density in solution	solNitrAcid	8 sets	8 sets	8 sets
Total density of solution	solRhoGes	8 sets	8 sets	8 sets

Table IV. Overview of the values and experimental uncertainties of tank parameters.

Parameter		Value	Uncertainty set 1	Uncertainty set 2
Outer solution radius				
Experiments	001, 002	13.96	0.190	0.078
	003, 004	14.005	0.070	0.029
	005-009	16.505	0.125	0.051
	010	25.345	0.625	0.255
Tank sidewall thickness				
Experiments	001,002	41.6	0.135	0.0805
	003, 004	41.9	0.018	0.013
	005-009	49.5	0.018	0.013
	010	30.9	0.018	0.013
Tank bottom wall thickness				
Experiments	001,002	0.64	0.114	0.071
	03-010	0.64	0.051	0.034

Table V. Overview of the values and experimental uncertainties of solution parameters.

Exp.	$\rho_{sol,U}$ [g/l]	σ_ρ [g/l]		$\rho_{solNitrAcid}$ [g/cm^3]	σ_ρ [g/l]		ρ_{solGes} [g/cm^3]	σ_ρ [g/cm^3]	
	value	set 1	set 2	value	set 1	set 2	value	set 1	set 2
001	145.68	1.04	1.05	0.294	0.002	0.0109	1.2038	0.0001	0.0025
002	346.73	0.95	2.25	0.542	0.005	0.0201	1.48	0.0003	0.0025
003	142.92	0.52	1.03	0.283	0.003	0.0105	1.2007	0.0024	0.0025
004	357.71	1.99	2.33	0.549	0.015	0.0203	1.4951	0.0006	0.0025
005	54.89	0.25	1.26	0.105	0.001	0.0039	1.0758	0.0006	0.0025
006	59.65	0.42	1.37	0.114	0.004	0.0042	1.0825	0.0006	0.0025
007	137.4	0.63	0.99	0.287	0.002	0.0106	1.1923	0.0007	0.0025
008	145.68	1.04	1.05	0.294	0.002	0.0109	1.2038	0.0001	0.0025
009	357.71	1.99	2.33	0.549	0.015	0.0203	1.4951	0.0006	0.0025
010	63.95	0.34	1.47	0.111	0.003	0.0041	1.0883	0.0002	00025

The uncertainties of the impurities of the tank materials, the effect of the paint layer on the tank and the effect of impurities in the solutions were neglected.

The calculated values for the energy of average lethargy causing fissions (EALF) show three distinct groups: experiments 002, 004 and 009 have values between 0.25 and 0.29, experiments 005, 006 and 010 have values between 0.042 and 0.045, while all other experiments (001, 003, 007 and 008) lie between 0.078 and 0.080.

4. UNCERTAINTY ANALYSIS (K_{eff})

Figure 1 shows the calculated k_{eff} values and their uncertainties. In blue the benchmark k_{eff} values including the reported experimental error bars of k_{eff} are shown. In purple an example calculation from [1] performed with KENO and a 27-energy group library based on ENDF/B-V is shown. Green and red shows the two GRS calculations with the resulting uncertainties using uncertainty set 1 and 2. Blue and orange show the ORNL calculations with their uncertainties for both uncertainty sets.

All our new calculations underestimate k_{eff} slightly, but are in good agreement with the experimental values within the error bars. In contrast to that the reported calculation (purple dots) overestimate k_{eff} and mostly lie outside of the 1-σ intervals.

Both the GRS – set 1 (green) and the ORNL – set 1 (light blue) reproduce the given experimental uncertainties (dark blue) quite well, while sets 2 of both institutions underestimate the experimental values.

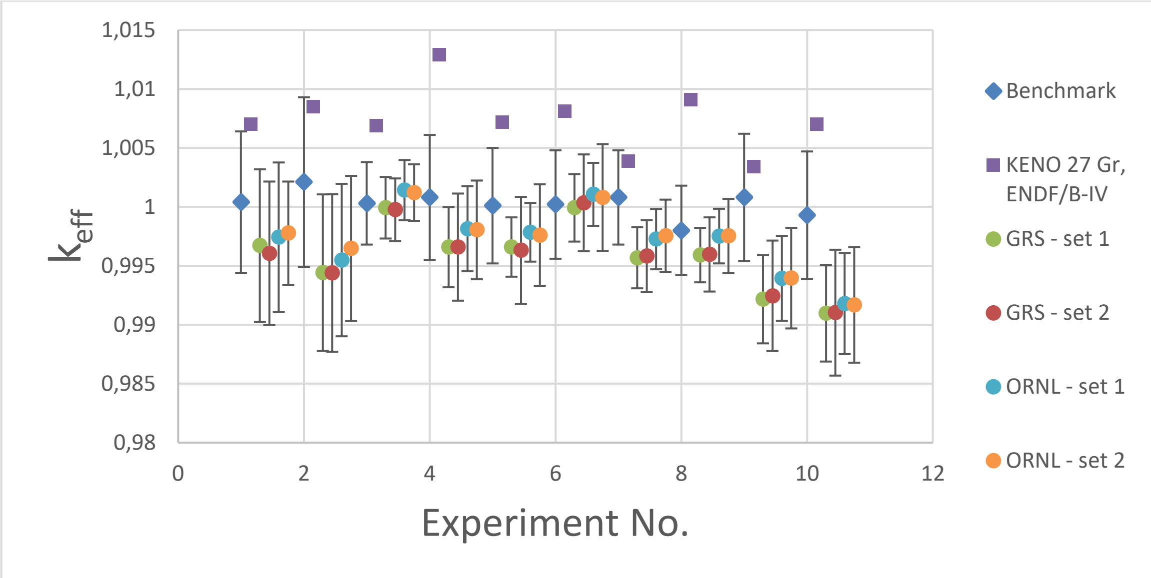

Figure 1. k_{eff} values of all calculated cases

5. CORRELATION ANALYSIS

From the sampled k_{eff} calculations the Pearson correlation between the benchmark experiments can be calculated. Figure 4 shows the matrices for all experiments for the two sets of data and for the independent calculations of GRS and ORNL. In comparison the correlation matrix extracted from DICE [5] is shown.

The plots in Figure 2 show several noteworthy features. For uncertainty set 1 some distinct features can be observed in the data:

- Experiments sharing the same tank are correlated with each other: 001/002, 003/004, and 005 to 009. However, the degree of correlation has a large spread from 0.33 to 0.97.
- Sharing the same solution parameters can lead to significant correlations (004/009), but it does not have to (001/008).
- Experiments which share neither the tank nor the solution have no statistically significant correlation coefficients.

For uncertainty set 2, almost all experiments are uncorrelated. Only two stronger correlations can be observed.

- Experiments 001 and 002 have a higher correlation due to the relatively high uncertainty of the steel tank dimension.
- Experiment 004 and 009 show higher correlation due to correlated solution parameters.

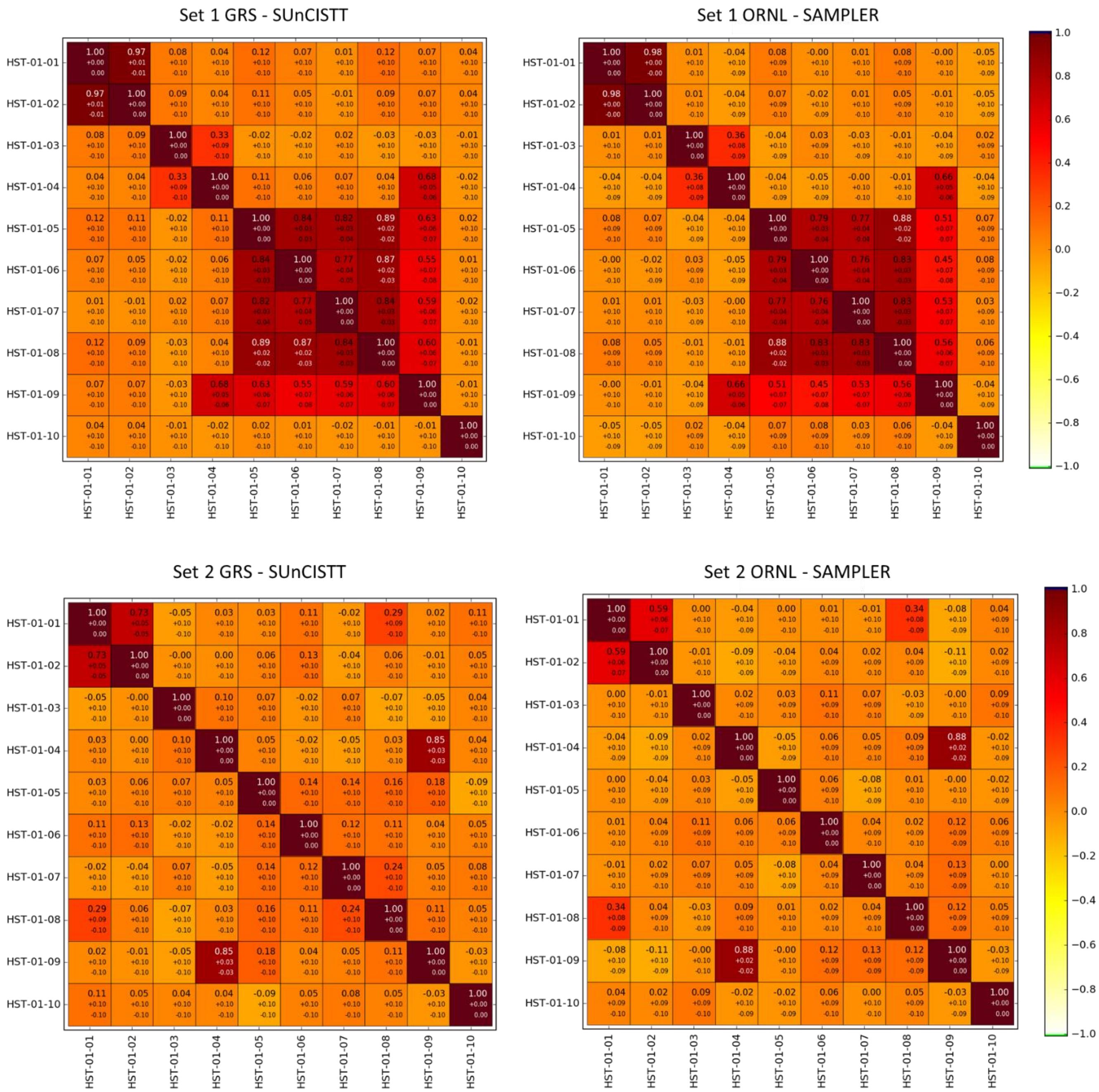

Figure 2. Pearson correlation matrices and the upper and lower 1.96 σ values for all experiments and for both sets of uncertainties calculated with SUnCISTT and SAMPLER

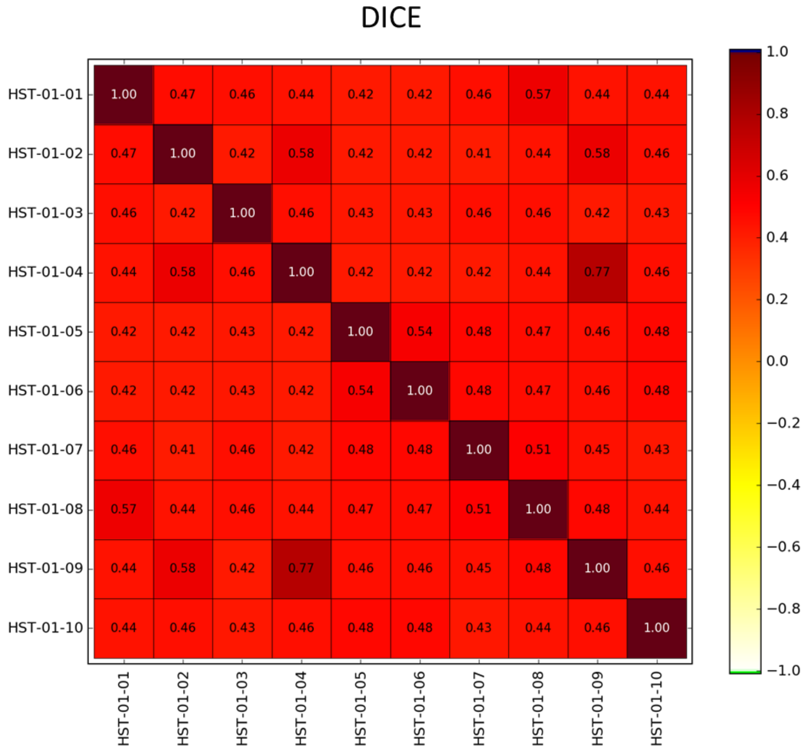

Figure 3. Pearson correlation coefficients for all experiments taken from DICE

The calculations of GRS and ORNL show for both sets of uncertainties identical correlation coefficients within their uncertainties. Note that the calculations were done completely independent from the extraction of uncertainties from literature, input generation up to the used uncertainty tool (SUnCISTT vs. SAMPLER) and the calculation of the Pearson correlation factors. This shows that the methodology of creating correlations factors works and is robust.

However, it also shows that the interpretation of the experimental data remains the crucial point in the entire endeavor. Depending on the used data in the same and accepted benchmark description in the ICSBEP handbook, completely different correlation matrices are produced.

Comparing the low confidential correlation factors form DICE with the two sets of data analyzed in this work, shows an even different picture. A more or less equal correlation (around a value of 0.5) is given for all experiments. Only experiments 004/009 show a higher correlation, as also observed with our calculations.

These features depend on the modelling assumptions. Especially all solutions with different densities are assumed to be completely independent, since no information is available, how these solutions are mixed together: If a ready solution is diluted further and further (which would imply further correlations), or if every solution is mixed individually from basic ingredients.

6. SENSITIVITY ANALYSIS

A sensitivity analysis on the varied parameter was performed. Therein the Pearson correlation factors between all varied technical parameter and the calculated k_{eff} for all experiments were calculated. Note that this is not a classical sensitivity but gives a measure for the impact of the actual variation of each parameter on the uncertainty of k_{eff}. Figure 4 shows the results for both sets of uncertainty for the GRS calculations.

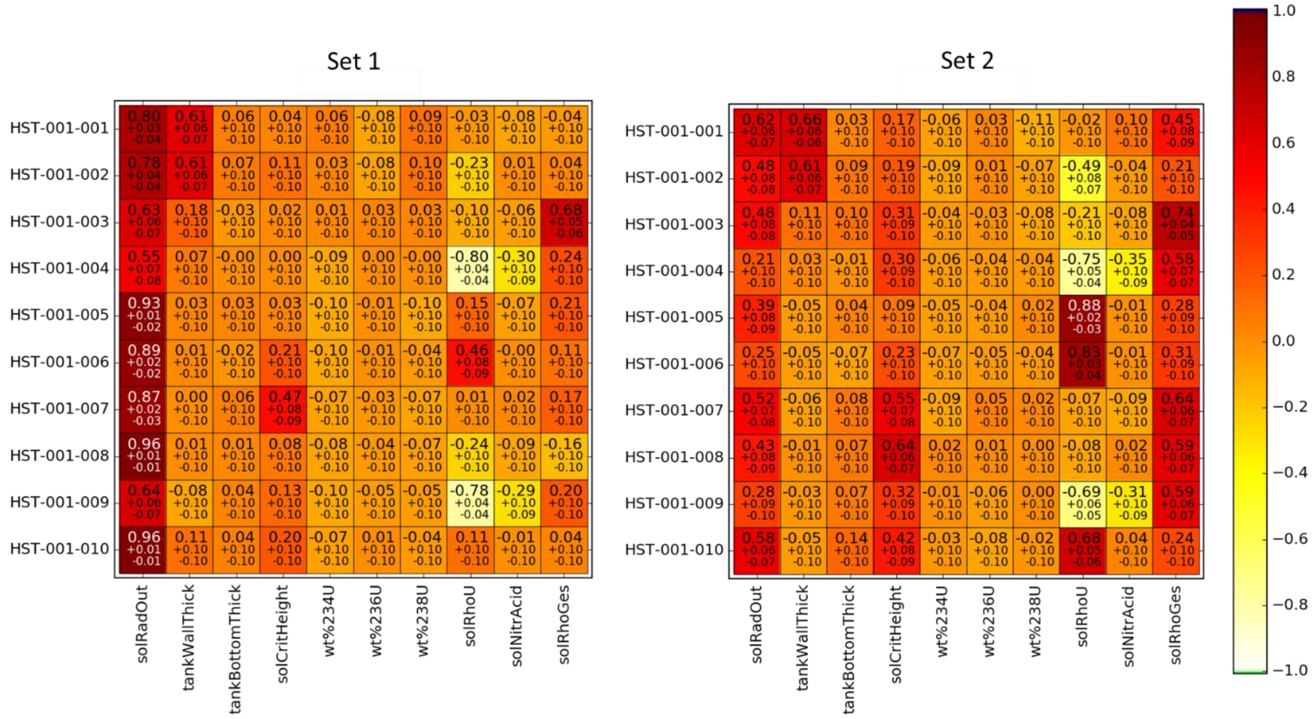

Figure 4. Correlation coefficients and the upper and lower 1.96 σ values between all varied technical parameters and k_{eff}.

From Figure 4 some significant differences can be observed between the two sets of uncertainty. Depending on the experiment and the set of used uncertainties, different uncertain technical parameters have a different impact on k_{eff}. The sensitivity of k_{eff} on the uranium concentration reflects the calculated EALF values. The negative correlations between the uranium density of experiment 002, 004 and 009 with k_{eff} show an under-moderation of these systems (high EALF). The positive correlations of experiment, 005, 006 and 010 show an over-moderation. The next to zero correlation of experiment 001, 003, 007 and 008 show a near optimal moderation.

While for set 1 the outer solution radius has the largest impact on k_{eff} for most of the experiments, its importance is less pronounced for set 2.

This sensitivity plot also explains the different correlations between experiment 001/008 and 004/009. While k_{eff} of the first pair is basically only sensitive on geometrical quantities which are independent for the experiments the second pair is also sensitive on the uranium, nitric acid, and total density due to a different moderation regime. Accordingly, a correlation between the second pair arises while the first pair remains uncorrelated.

The strong correlation between experiment 001 and 002 can be explained by the similar sensitivity of both experiments to the variation of the outer solution radius and the tank wall thickness. These two are basically the only quantities, on which k_{eff} is sensitive to.

7. CONCLUSIONS

In this work we presented a detailed sensitivity, uncertainty, and correlation study of k_{eff} values with focus on uncertain technical parameters of ten experiments of critical high enriched uranium solutions with a thermal neutron spectrum. The total Monte Carlo approach was chosen to allow all uncertain quantities to be sampled at once following their individual distribution functions. The stochastic dependencies between variables of different experiments were chosen according to the available data.

The analyses were done individually and independent by GRS using the code SUnCISTT [2] and ORNL using the SCALE sequence SAMPLER [3]. Both Monte Carlo approaches rely on the neutron transport code KENO from SCALE 6.2.2 [4]. This enables a direct comparison of the implemented Monte-Carlo methods. The resulting keff-values and Pearson´s correlation coefficients for the uncertainty sets 1 and 2 are in excellent agreement and the correlation coefficients statistically identical.

The two codes were used to analyze two different sets of uncertainties, both given in different chapters of the ICSBEP handbook description of the HEU-SOL-THERM-001 series. The different uncertainties given for the two evaluations lead to some significantly different values in the correlation matrices and differences in the sensitivities. The correlation coefficients for experiments 005 to 009 are significantly different for the two uncertainty sets. They vary from no correlation for set 2 to correlation coefficients of order 0.6 to 0.8 for set 1. Producing reliable correlation coefficients based on the uncertainties given in the ICSBEP would imply to preliminarily discuss different uncertainty evaluations. However, the two codes SUnCISTT and SAMPLER deliver statistically identical results assuming the same uncertainty sets.

A comparison with the correlation coefficients given in DICE [5] shows a significant deviation to the results generated in this work. Basically, all coefficients for HST-001 in DICE are around 0.4 to 0.5 (except for 004/009). The full Monte-Carlo analysis revealed different values. For the uncertainty set 1 almost all experiments are not correlated, except for experiments 001/002, 001/008 and 004/009. Applying uncertainty set 2 leads to a more structured correlation matrix with several experiments being correlated. This shows, that the coefficients given in DICE should be handled with care.

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REFERENCES

[1] OECD-NEA,"International handbook of evaluated criticality safety benchmark experiments," Tech. Rep. **NEA/NSC/DOC(95)03**, NEA Nuclear Science Committee, 2016.

[2] M. Behler, M. Bock, F. Rowold and M. Stuke, "SUnCISTT - A Generic Code Interface for Uncertainty and Sensitivity Analysis", Probabilistic Safety Assessment and Management PSAM12, Honolulu, Hawaii, USA, 22-27 June, (2014).

[3] B. T. Rearden, K. J. Duggan and F. Havluj, "Quantification of Uncertainties and Correlations in Criticality Experiments with SCALE," ANS Nuclear Criticality Safety Division Topical Meetings (NCSD2013), Wilmington, NC, 2013.

[4] B.T. Rearden and M.A. Jessee, Editors, "SCALE Code System", **ORNL/TM-2005/39**, Version 6.2, Oak Ridge National Laboratory, Oak Ridge, TN (2017).

[5] OECD-NEA: "Database for the International Criticality Safety Benchmark Evaluation Project (DICE)", September 2015 Edition, build 2.7, 2015.

[6] M.B. Chadwick et al., "ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data", NuclearData Sheets, 112, pp. 2887-2996, 2011.

[7] F. Sommer and M.Stuke, "Convergence of Correlation Coefficients of Critical Experiments Derived by Monte Carlo Sampling", Proc. NCSD Topical Meeting 2017, Carlsbad, New Mexico, USA, 2017.