Use of International Criticality Safety Benchmark Evaluation Project Benchmarks for the Validation of CSAS26 (Scale 4.4a) for Configurations of Low-Enriched Uranium

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Abstract — *As an example of the application of the International Criticality Safety Benchmark Evaluation Project (ICSBEP) work to the nuclear industry, the validation of the control module CSAS26 of SCALE 4.4a for criticality calculations on a personal computer platform is presented. This work has been done using the models of critical experiments being compiled by the Organisation for Economic Co-operation and Development/Nuclear Energy Agency (OECD/NEA) since 1992. The description and results of this compilation were first presented during the Fifth International Conference on Nuclear Criticality Safety (ICNC'95). Out of 2881 critical configurations included in the latest edition (September 2002) of the ICSBEP "International Handbook of Evaluated Criticality Safety Benchmark Experiments," NEA/NSC/ DOC(95)03, OECD/NEA, 131 have been selected for the CSAS26 validation. The selected critical experiments have characteristics similar to the systems to be simulated with CSAS26 for low-enriched uranium (LEU) fuel fabrication applications. They represent both homogeneous configurations and hexagonally pitched rod lattices of low-enriched (from 1.60 to 5.00 wt% ^{235}U) UO_2 with several absorbers. The statistical uncertainties related to the application of CSAS26 for criticality calculations are also evaluated. The great number of cases involved allows an exhaustive statistical treatment of the data, including the analysis of correlations related to the type of system being simulated. The statistical uncertainties found are very small. As a result, the module CSAS26 is considered as a quite suitable calculational method for application to criticality safety analysis at LEU facilities.*

I. INTRODUCTION

As established in the standard ANSI/ANS-8.1-1998 (Ref. 1), any calculational method used to analyze the behavior of systems containing fissionable material has to be validated to determine the bias and related uncertainties. This process allows normalization of the method within its range of applicability in such a way that it is able to correctly predict criticality conditions within the limits of the uncertainties related both to the bias and to the k_{eff} of each particular case. Thus, the present paper presents the results and methodology applied for the validation of the control module CSAS26 (BONAMI/ NITAWL-II/KENO-VI) of SCALE 4.4a to execute criticality calculations on a personal computer platform.

One of the most commonly used validation strategies consists of simulating critical configurations by using the calculational method intended to be validated and comparing the results to the previously known experimental values. Following this approach and starting with the experimental data from Ref. 2, the next sections of this paper present the results obtained from the simulation of 131 critical configurations performed using the control module CSAS26 with the 44-group library ENDF/B-V. Calculations were executed on a Pentium II/450-MHz machine with Windows NT 4.0 Terminal Server OS. Afterward, these results are compared to the benchmark value of each critical configuration, thus obtaining the bias of the method and the related statistical uncertainties.

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II. SELECTION OF THE EXPERIMENTAL MATRIX

Since 1992, the Organisation for Economic Co-operation and Development/Nuclear Energy Agency has assembled a huge compilation of critical experiments whose description and results were first presented during the Fifth International Conference on Nuclear Criticality Safety, held at Albuquerque, New Mexico, in September 1995. This compilation is included with a standardized format in Ref. 2 and constitutes a valuable tool for the validation of calculational methods used for criticality safety assessment purposes.

Out of 2881 critical experiments included in the latest edition of Ref. 2 (September 2002), 131 have been selected for this work. The selection criteria rely on fitting the experimental features to those of the systems to be simulated with CSAS26 in low-enriched uranium (LEU) fuel fabrication applications and, in particular, to the different configurations applicable to VVER designs during both the ceramic and mechanical stages of the fabrication process. Thus, the selected experimental matrix covers thermal, homogeneous, and heterogeneous configurations (hexagonally pitched lattices of rods) of low-enriched UO_2 (from 1.6 to 5.0 wt% ^{235}U) with light water moderation and in the presence of several burnable absorbers, such as B, Eu, or Gd.

II.A. VVER Experiments, KFKI (Budapest)

Between 1972 and 1990, the VVER-design user countries established a Temporary International Collective (TIC), led by Hungary, with the objective of performing joint experiments and code development in the scope of such fuel design. The experimental basis of TIC was the critical assembly ZR-6(M), operated by the Central Research Institute for Physics of the Hungarian Academy of Sciences (KFKI, Budapest).[3,4]

The experimental configurations studied in the ZR-6(M) critical assembly used UO_2 rods of several enrichments, between 1.60 and 4.40 wt% ^{235}U. In some cases, these configurations included different types of absorber rods (with B, Eu, or Gd) and different concentrations of H_3BO_3 dissolved in the moderator (light water). By changing these parameters, as well as the geometry of the configurations or their temperature, up to a total of 334 configurations were studied, 165 of which are included in Ref. 3 and 69 of which are included in Ref. 4. In all of them, criticality was achieved by modifying the level of the water.

Out of the total number of critical configurations included in Refs. 3 and 4, 98 have been selected for the validation of CSAS26. They can be classified into the following categories:

Category 1. regular lattices (group LCT15A, cases 1 through 55 of Table I), which are those

containing only UO_2 rods of the same enrichment[3]; see Fig. 1

Category 2. regular lattices with mixed enrichment (group LCT15B, cases 56, 57, and 58 of Table I) (Ref. 3). Figure 2 shows a typical scheme of the cross section for this lattice's category. Note how rods of a second enrichment are distributed around a regular lattice making a cylindrical envelope.

Category 3. lattices with point perturbations (groups LCT15C, cases 59 through 77 and LCT36, cases 80 through 98 of Table I), built up from regular lattices in which some UO_2 rods have been substituted by holes or absorber rods[3,4] (Fig. 3)

Category 4. combinations of categories 1 and 2 (group LCT15D, cases 78 and 79 of Table I) (Ref. 3). Figure 4 shows a typical scheme. The two main zones of different enrichment are clearly identified as well as the location of holes and absorber rods in the central area of the configuration.

II.B. Regular Lattices of U(5%)O2, RRC KI (Moscow)

In 1961, a series of critical experiments involving hexagonally pitched lattices of cylindrical rods with low enrichment (~5 wt% ^{235}U) was performed in the Russian Research Center "Kurchatov Institute" (RRC KI). These lattices were moderated by light water with or without H_3BO_3 (Refs. 5, 6, and 7). Criticality was achieved by changes in the total number of rods, the pitch, or the level of the water.

Out of 16 configurations included in Refs. 5, 6, and 7, 15 were selected for the validation of CSAS26. Attending to the type of cladding, the selected lattices can be classified into the following categories:

Category 1. lattices with stainless steel cladding (group LCT19, cases 99 and 100 of Table I) (Ref. 5)

Category 2. lattices with zirconium cladding (groups LCT20, cases 101 through 107 and LCT31, cases 108 through 113 of Table I) (Refs. 6 and 7).

All these 15 lattices follow similar schemes as those shown in Fig. 1.

II.C. MARACAS Program: Homogeneous U(5%)O2 Powder Configurations, IPSN (Valduc)

This set of experiments was carried out between 1983 and 1987 in a critical facility at Valduc, France, run by

TABLE I
Summary of Results

Group (Reference)	$I_{exp(i)}$	Case	Configuration	$k_{m(i)}$	$\sigma_{m(i)}$
LCT15A (3)	0.0030	1	175/175	0.9994	0.0014
		2	174/174	1.0012	0.0015
		3	154/154	0.9950	0.0014
		4	246/246	0.9977	0.0014
		5	173/173	0.9978	0.0014
		6	52/23	0.9973	0.0014
		7	172a/172	0.9994	0.0016
		8	51/24	0.9977	0.0015
		9	171a/171	0.9978	0.0015
		10	170/170	0.9972	0.0014
		11	169/169	0.9980	0.0013
		12	158/155	0.9945	0.0015
		13	162/161	0.9947	0.0014
		14	161/161	1.0019	0.0013
		15	163/161	0.9981	0.0014
		16	247/247	1.0039	0.0012
		17	195/39	0.9953	0.0014
		18	194/194	0.9924	0.0014
		19	193/193	0.9953	0.0013
		20	192/192	0.9968	0.0013
		21	188/40	0.9927	0.0013
		22	191/191	0.9930	0.0013
		23	212/212	0.9991	0.0016
		24	213/213	0.9984	0.0014
		25	214/214	1.0012	0.0017
		26	220/220	0.9977	0.0016
		27	215/215	0.9978	0.0015
		28	216/216	0.9960	0.0016
		29	217/217	1.0015	0.0013
		30	218/218	0.9989	0.0014
		31	219/219	1.0002	0.0015
		32	233/233	1.0034	0.0013
		33	232/232	1.0029	0.0014
		34	234/234	1.0019	0.0012
		35	235/235	1.0120	0.0013
		36	236/236	1.0020	0.0013
		37	237/237	1.0046	0.0013
		38	230/230	0.9968	0.0013
		39	229/229	0.9977	0.0015
		40	225/225	0.9972	0.0016
		41	221/221	1.0010	0.0016
		42	224/224	1.0013	0.0017
		43	223/223	0.9965	0.0019
		44	208/208	1.0060	0.0013
		45	207/207	1.0026	0.0015
		46	206/206	1.0060	0.0016
		47	205/205	1.0032	0.0013
		48	204/204	1.0055	0.0015
		49	203/203	1.0049	0.0014
		50	202/202	1.0015	0.0015
		51	201/201	1.0029	0.0015
		52	200/200	1.0033	0.0016
		53	199/199	1.0030	0.0013
		54	110/110	0.9959	0.0015
		55	164/110	0.9943	0.0014
LCT15B (3)	0.0030	56	160/160	0.9960	0.0014
		57	166/166	0.9956	0.0015
		58	231/231	0.9952	0.0012

Group (Reference)	$I_{exp(i)}$	Case	Configuration	$k_{m(i)}$	$\sigma_{m(i)}$
LCT15C (3)	0.0030	59	158-1/155	0.9922	0.0017
		60	158-2/155	1.0000	0.0016
		61	158-3/155	0.9974	0.0015
		62	158-4/155	0.9944	0.0013
		63	158-5/155	0.9981	0.0018
		64	158-6/155	0.9979	0.0014
		65	158-7/155	0.9984	0.0016
		66	155/155	1.0084	0.0013
		67	155-1/155	1.0046	0.0015
		68	156/155	1.0012	0.0016
		69	244/244	1.0002	0.0014
		70	243/243	0.9995	0.0015
		71	156-1/155	0.9974	0.0016
		72	1244/244	0.9939	0.0014
		73	157/155	0.9962	0.0016
		74	245/244	0.9932	0.0014
		75	189/189	0.9941	0.0013
		76	242/242	1.0022	0.0015
		77	190/190	0.9995	0.0016
LCT15D (3)	0.0030	78	197/197	1.0044	0.0015
		79	198/198	1.0036	0.0013
LCT36 (4)	0.0090	80	293/293	0.9974	0.0014
		81	294/294	0.9982	0.0016
		82	295/295	0.9946	0.0016
		83	296/296	0.9932	0.0015
		84	297/297	0.9964	0.0017
		85	298/298	0.9952	0.0017
		86	299/299	0.9975	0.0014
		87	302/302	0.9940	0.0015
		88	303/303	0.9969	0.0016
		89	304/304	0.9950	0.0016
		90	305/305	0.9968	0.0017
		91	306/306	0.9988	0.0015
		92	307/307	0.9975	0.0016
		93	308/308	0.9981	0.0016
		94	309/309	0.9927	0.0015
		95	310/310	0.9973	0.0016
		96	311/311	0.9949	0.0015
		97	312/312	0.9976	0.0018
		98	313/313	0.9952	0.0014
LCT19 (5)	0.0058	99	2	1.0062	0.0018
	0.0061	100	3	1.0054	0.0012
LCT20 (6)	0.0061	101	1	0.9972	0.0013
		102	2	0.9998	0.0015
		103	3	1.0029	0.0015
		104	4	1.0033	0.0016
		105	5	1.0018	0.0014
		106	6	1.0039	0.0015
		107	7	1.0043	0.0014
LCT31 (7)	0.0045	108	1	0.9880	0.0014
		109	2	0.9912	0.0016
		110	3	0.9939	0.0019
		111	4	0.9895	0.0015
		112	5	0.9909	0.0016
		113	6	0.9933	0.0014

(Continued)

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TABLE I (Continued)

| Group (Reference)	$I_{exp(i)}$	Case	Configuration	$k_{m(i)}$	$\sigma_{m(i)}$
LCT49 (8)	0.0034	114	R2-2R(6,6)	1.0004	0.0015
		115	R1-3R(6,6)	1.0020	0.0013
		116	R2-3R(6,6)	1.0002	0.0016
		117	R3-3R(6,6)	1.0027	0.0014
	0.0042	118	R2-2R(4,5)	0.9971	0.0015
		119	R1-3R(4,5)	1.0005	0.0013
		120	R1-2R(5,5)	1.0008	0.0018
		121	R2-2R(5,5)	1.0004	0.0013
	0.0037	122	R2-2R(4,3)	0.9982	0.0013
		123	R1-3R(4,3)	1.0003	0.0015
		124	R1-2R(4,4)	0.9981	0.0015
		125	R2-2R(4,4)	0.9994	0.0014
	0.0036	126	R2-3R(4,4)con	1.0037	0.0015
		127	R3-3R(4,4)con	1.0028	0.0016
		128	R2-4R(4,4)con	0.9974	0.0014
		129	R1-2R(5,5)che	0.9999	0.0015
		130	R2-2R(5,5)che	0.9999	0.0015
	0.0030	131	R2-1R(3,3)mod	1.0017	0.0014
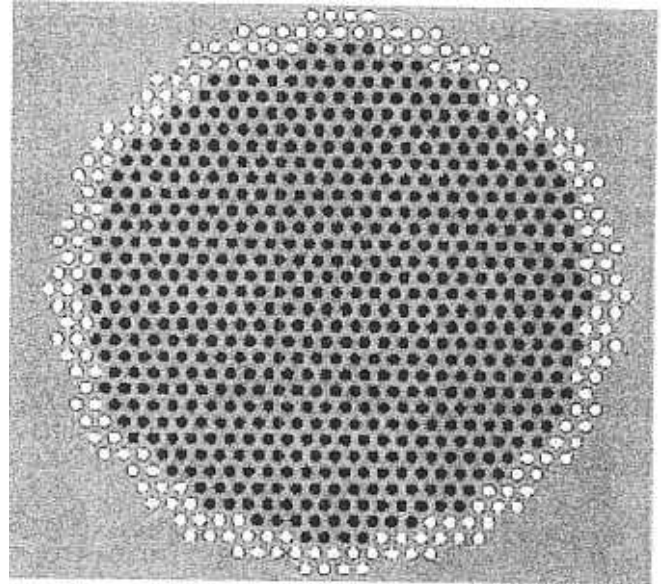
Fig. 2. Mixed-enrichment lattice cross section.

the Safety and Criticality Research Service of the Institute of Nuclear Protection and Safety (IPSN). The experimental basis of this program was the split-table testing device called "MARACAS" (Ref. 8). The experiments included involved low-water-moderated and low-enriched (5 wt% ^{235}U) uranium dioxide powder assemblies with polythene reflection. These assemblies consisted of boxes
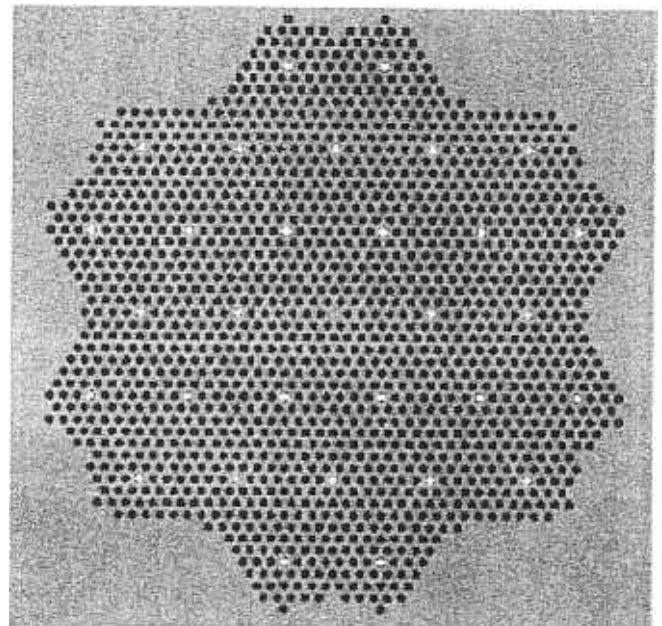

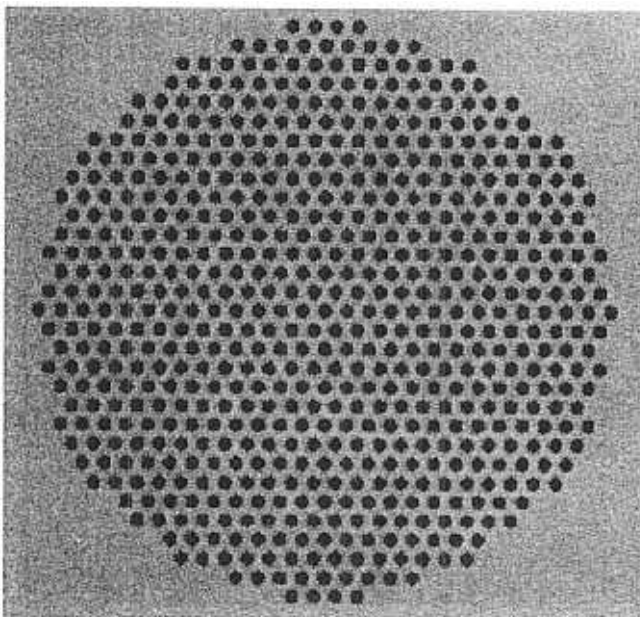Fig. 3. Cross section of a lattice with point perturbations.

filled with moistened UO_2 powder that were stacked on one of the two halves of the MARACAS device. All the experiments were subcritical approaches extrapolated to critical by measuring distances between the two halves of the split table.

All 18 configurations included in Ref. 8 were chosen for the CSAS26 validation. They comprised the group LCT49 of Table I and can be classified as follows:

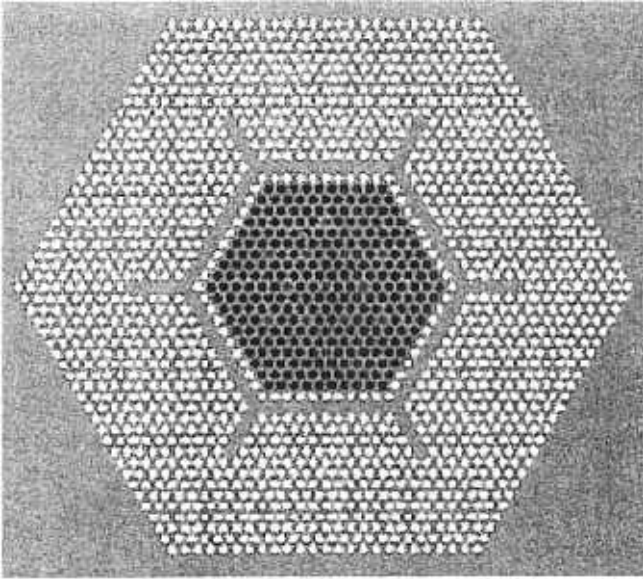Fig. Regular lattice cross section.

Fig. 4. Cross section of category 4 lattice type on p. xxx

1. configurations with the same H/U ratio, equal to 2.0 (cases 114 through 117), 2.5 (cases 118 through 121), or 3.0 (cases 122 through 125)

2. configurations with mixed H/U ratio, assemblies with both boxes of H/U = 2.0 and H/U = 3.0 together, arranged in concentric layers (cases 126, 127, and 128) or as a checkerboard (cases 129 and 130)

3. modular configuration, comprising boxes with H/U ratios of 2.0 and 3.0, empty boxes and boxes with absorber crossing blades (case 131).

III. ANALYSIS OF THE RESULTS

The selected 131 critical experiments have been simulated by means of CSAS26 with the 44-group library ENDF/B-V. As a result of this simulation, the multiplication factors $k_{m(i)}$ ($i = 1,...,131$) shown in Table I are obtained, along with their respective errors of the mean, designated as $\sigma_{m(i)}$. A total of 250 generations of 1500 neutrons each were run for each calculation. In order to minimize the variance of the results, the first 50 generations were skipped in all calculations. These are the values of $k_{m(i)}$ and $\sigma_{m(i)}$ that are included in Table I.

In all cases, the experimental value of k_{eff} is assumed to be 1.0000 as specified in the original references, though its accuracy depends on the configuration. Thus, the experiments performed under similar conditions are grouped in Table I. The accuracy $I_{exp(i)}$ of the experimental k_{eff} from the reference for each group of similar experiments is also indicated in Table I. The col-

umn "Configuration," which is the identification of the configuration in the original references, is included to link each case with its related experimental configuration.

The standard ANSI/ANS-8.17-1997 (Ref. 9) gives guidance to determine an upper subcritical limit (USL) from the bias and uncertainties related to the calculational method being used. More specifically, Ref. 9 states that to assure subcriticality by computing the neutron multiplication factor k_p of a particular system, the following expression shall be fulfilled:

$$k_p + |\Delta k_p| \leq USL = k_c - |\Delta k_c| - |\Delta k_m| , \qquad (1)$$

where

k_c = mean k_{eff} that results from the simulation of critical experiments using the code intended to be validated

Δk_c = uncertainty in the determination of k_c

Δk_p = uncertainty related to the computation of k_p

Δk_m = (arbitrary) value required to ensure an acceptable margin of subcriticality.

Note that expression (1) can be rewritten as

$$k \equiv k_p + (1 - k_c) + |\Delta k_c| + |\Delta k_p| \leq 1 - |\Delta k_m| , \qquad (2)$$

which allows one to define k, the maximum allowable value for the k_{eff} of the system subjected to study as a function of the required Δk_m.

The values of k_c and Δk_c must be estimated from the results of the simulation of critical experiments. Checks on correlations of the results related to the different parameters taken into account (enrichment, pitch, etc.) in the simulated systems were carried out; no trends were observed. Thus, all 131 cases in Table I are considered as an unique sampling group and were checked for normality applying the D' test as recommended by Ref. 10 when the sample size $n > 50$. Once normality of the population is assumed, the estimator of k_c can be computed using the arithmetic mean of the individual $k_{m(i)}$:

$$\bar{k}_c = \frac{\sum_{i=1}^{n} k_{m(i)}}{n} , \qquad (3)$$

where $n = 131$. The term Δk_c is then computed from the sample variance

$$s_c^2 = \frac{\sum_{i=1}^{n} (k_{m(i)} - \bar{k}_c)^2}{n - 1} \qquad (4)$$

and the internal variance of the data σ_c^2, determined from the quadratic means of the deviations $\sigma_{m(i)}$ and of the uncertainties $I_{exp(i)}$. The reference papers included in Ref. 2 describe the confidence levels used to calculate the experimental uncertainty only for cases 114 through

131, for which $I_{exp(i)} = 3\sigma_{exp(i)}$ (Ref. 8). For the rest of the cases, it is assumed that the experimental uncertainties are given for a centered interval and at a 95% confidence level.[11] That is, for $i = 1, \ldots, 113, I_{exp(i)} = 2\sigma_{exp(i)}$ is taken. Then,

$$\sigma_c^2 = \frac{1}{n} \sum_{i=1}^{n} \sigma_{m(i)}^2 + \frac{1}{n} \left(\sum_{i=1}^{113} \frac{I_{exp(i)}^2}{4} + \sum_{i=1,4}^{131} \frac{I_{exp(i)}^2}{9} \right) \quad (5)$$

Taking into account the rule for the addition of variances of statistically independent random variables, we have

$$|\Delta k_c| = K_c \sqrt{s_c^2 + \sigma_c^2} \ , \quad (6)$$

where the coverage factor K_c depends on the significance level (i.e., probability) $P = 1 - \alpha$ desired to compute k_c. Applying the criteria established in the standard,[12] the USL must be determined as a 95/95 one-sided tolerance limit. Mathematically, the problem is to find a K_c such that

$$\Pr\{\Pr(X \le \bar{x} + K_c s) \ge P\} = \gamma \ , \quad (7)$$

where X follows a normal distribution and P and γ are the specified probabilities, both equal to 0.95. Then, K_c is the quantile verifying

$$\Pr\{T_f \le K_c \sqrt{n} \,|\, C_p \sqrt{n}\} = \gamma \ , \quad (8)$$

where T_f is the noncentral $- t$ Student's distribution with $f = n - 1$ degrees of freedom and C_p is the $z_{1-\alpha}$ value of the standard normal distribution. In our case $f = 130$, $\alpha = 0.05$, and $\gamma = 0.95$. Upon these conditions, $K_c = 1.888$.

The term Δk_p, related to the calculation uncertainty of a particular case, is determined from the calculation error σ_p for the estimator $\bar{k}_p$ of the k_{eff} of the actual case. Both values are supplied by CSAS26. This uncertainty is computed by multiplying σ_p by the coverage factor K_p related to the desired significance level. Taking into consideration that both $\bar{k}_p$ and σ_p are computed after a large number of Monte Carlo generations (250 at least) whose k_{eff}'s follow a normal distribution, the upper limit of the one-sided γ confidence interval of the estimator $\bar{k}_p$ is given taking $K_p = z_{1-\alpha}$, where $z_{1-\alpha}$ is the quantile of the standard normal distribution corresponding to the desired confidence level. If $\alpha = 0.05$, $z_{0.95} = 1.645$. Conservatively, $K_p = 2$ is assumed, and thus, $|\Delta k_p| = 2\sigma_p$.

This new term must be added to Eq. (6) following the variance's addition rule, which leads to

$$|\Delta k_p| + |\Delta k_c| = \sqrt{K_p^2 \sigma_p^2 + K_c^2(s_c^2 + \sigma_c^2)} \ , \quad (9)$$

which allows rewriting Eq. (2) as

$$k = k_p + (1 - k_c) + \sqrt{K_p^2 \sigma_p^2 + K_c^2(s_c^2 + \sigma_c^2)}$$

$$\le 1 - |\Delta k_m| \ . \quad (10)$$

TABLE II

Parameters $\bar{k}_c$, s_c^2, and σ_c^2

$\bar{k}_c$	s_c^2	σ_c^2	$s_c^2 + \sigma_c^2$
0.9988	1.6322E−05[a]	7.5635E−06	2.3886E−05

[a]Read as 1.6322×10^{-5}.

Table II shows the values of $\bar{k}_c$, s_c^2, and σ_c^2 resulting from the application of expressions (3), (4), and (5).

IV. CONCLUSIONS

Substituting the numerical values of the parameters in Eq. (10) and k_p and k_c by their estimators, the final expression, which compares the maximum allowable value for the k_{eff} of the system subjected to study with the required Δk_m, is obtained:

$$k = \bar{k}_p + 0.0012 + \sqrt{4\sigma_p^2 + 8.5142 \times 10^{-5}}$$

$$\le 1 - |\Delta k_m| \ , \quad (11)$$

where $\bar{k}_p$ and σ_p are the values supplied by CSAS26 for the k_{eff} of the particular system and for its standard deviation, respectively, and Δk_m is the additional (arbitrary) safety margin.

Finally, if the numerical values of Table II are substituted into Eq. (1), the expression for the USL as a function of Δk_m is obtained:

$$\text{USL} = 0.9896 - |\Delta k_m| \quad (12)$$

The results of the statistical approach described in this paper have been compared with the methodology stated in Ref. 13, which leads to the conclusion that both approaches give similar results. In fact, the USL, as stated by expression (12), is just 0.1% more conservative than the most pessimistic value obtained by means of the method described in Ref. 13, which gives an idea of how close the results obtained by both approaches are.

Expressions (11) and (12) stand for calculations performed with the 44-group ENDF/B-V library on systems with features similar to those of the critical configurations used for the present validation. Basically, such systems are thermal, homogeneous configurations and hexagonally pitched lattices of rods of LEU (enrichment below 5.0 wt% ^{235}U) with light water moderation. The uncertainties found are very small, so that CSAS26 is considered as a quite suitable calculational tool for application in LEU facilities.

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