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Validation of MORET 4 Perturbation against 'Physical' Type Fission Products Experiments

Dr. Jacques ANNO[1], Olivier JACQUET, Dr. Joachim MISS

Institut de Radioprotection et de Sûreté Nucléaire IRSN, BP 17, 92262 Fontenay aux Roses Cedex, France

After shortly recalling one among the many pertinent recent features of the French criticality CRISTAL[1)] package i.e. the perturbation algorithm (so called MORET 4 'Perturbation' or MP), this paper presents original MP validations. Numerical and experimental validations are made using close fission products (FP) experiments. As results, it is shown that, all being equal, MP can detect FP's absorption cross-section variations in the range 0.3 – 1.2 %.

1. Introduction

MORET 4 'Perturbation' (MP) is based on the Correlated Sampling Method (CSM) [2)]. It allows calculating easily, accurately, simultaneously and without an important increase of calculation time, the Keff of a benchmark and the effect in Keff difference (ΔK) of small perturbations on the data, especially atom densities and mixture concentration.

After other 2000 numerical various validation cases against deterministic Sn Keff differences, a new type of validation was recently performed using results of French critical FP experiments. The paper shortly recalls the CSM interest. Then numerical and experimental MP validations using FP benchmarks are presented. Taking into account the sensitivity of these MP validations, the detection limits of small absorption cross-section variation are determined.

2. Correlated Sampling Method

The keff difference of two independent Monte Carlo calculations ($keff = k_i \pm \sigma_i$, i = 1,2) is given by:

$$\Delta keff = k_1 - k_2 \pm \sqrt{(\sigma_1^2 + \sigma_2^2)} \quad (1)$$

The variance of the difference:

$$Var\,(k_1 - k_2) = \sigma_1^2 + \sigma_2^2 \quad (2)$$

is never null. On the contrary, when using CSM, one takes advantage of the variance of difference:

$$\sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2 = (\sigma_1 - \sigma_2)^2 - 2(1-\rho)\sigma_1\sigma_2 \quad (3)$$

with $-1 \leq \rho \leq +1$ being the correlation coefficient. This variance can be zero when $\rho \sim 1$ for two close systems. But, greater is the difference between the two calculated systems, lesser is the correlation and larger is the variance and the uncertainty on the calculated Δkeff. Thus, it is sometimes preferable to perform the neutron life Monte Carlo simulation process in an intermediary (reference) system, between the nominal and perturbed (modified) systems.

In MORET 4, perturbations can be made on systems having the same geometry, but varying by the chemical composition in one or more media.

Two perturbation types are possible:

- Changing one nominal chemical mixture by another,
- Changing the density of one nominal mixture.

Some geometrical perturbations are possible, when they can be considered and described as chemical perturbations.

MORET 4 can simultaneously manage 8 perturbed systems.

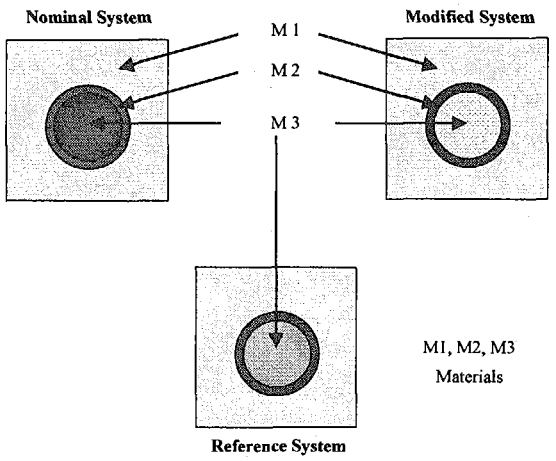

Fig. 1 Schematic Principle of a Perturbation

Results are keff values of the nominal system, calculated according 6 individual and 3 combined estimators and their related standard deviations, the asked Δkeff and its standard deviation σ for each perturbation, also according 6 individual and 3 combined estimators.

For checking the perturbation calculation rightness, MORET 4 also gives the correlation coefficients ρ and the asymptotic slope values of Δkeff probability density function for each individual Δkeff estimator.

[1] Corresponding author, Tel 33 1 58 35 81 15 Fax 33 1 46 57 29 98, E-Mail: jacques.anno@irsn.fr

During the implementation of the perturbation calculation in MORET 4, many numerical validation calculations were performed:

- 500 during the preparation phase on various fissile media, as UO_2 or PuO_2, in crystal or powder state, with 5 types of changing: density, isotopic, moderation ratio, small thickness variation of a fissile material, replacing small fissile thickness material by water.
- 1500 during the validity limits determination, by variation calculations on the most encountered cases in criticality calculations. Among them, 180 calculations cases were performed on critical experiments, such as for determining uncertainties weights of the published LEU-COMP-THERM-05 benchmark compared against deterministic calculation differences. Especially, it was shown that MORET 4 Perturbation is a very convenient, accurate, efficient and fast tool to determine uncertainties weights and parameters sensitivities of critical experiments.

3. Experimental Validation

3.1 Data Base

IRSN has a large database of French experiments made in Saclay and Valduc [3]. Recent Fission Products experiments are very accurate [4]. Refer to this publication for the description and some results, which principle is shortly described in the following Figure 2.

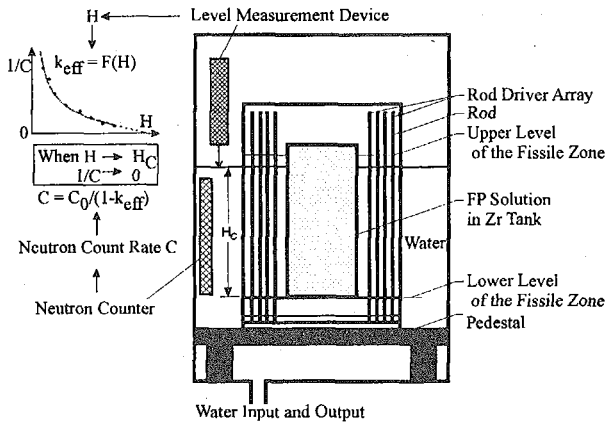

Fig. 2 Sub-critical Approach Principle: At each water level height H, neutron count rates C depend on Keff. When Keff increases towards 1, 1/C decreases to zero. Thus, the intersection with the abscissa of the extrapolated tangent of the curve 1/C = F(H) from the last measured points determines the critical level H_c.

In particular, experiments in the same driver array configurations (23x23-25 to 25x25-25, the latter 25 rods being removed for making place to the central tank) and the same fission product solution only differ by this fission product mixture in the central tank. They only differ on FP concentration and on solution acidity. Others differ on FP nature in slightly acidic aqueous solution.

3.2 Method

Thus the difference in water height ΔH, which is the sub-critical approach parameter, is correlated to Keff difference. With the relationships K=F(H) and its derivative, it is easy to obtain mathematically the ΔK value resulting from ΔH, when changing a mixture with another one for the same FP and the same geometry.

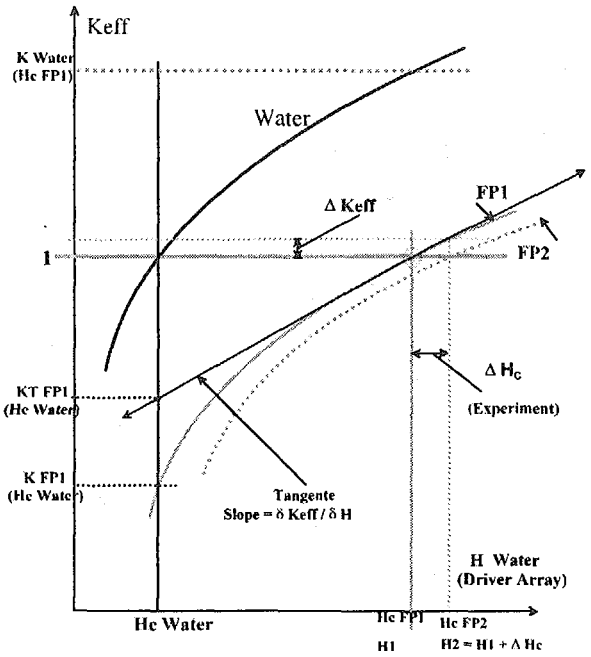

Fig. 3 Keff Variation against H Water (Driver Array) for the same Driver Array Geometry

The Figure 3 displays the principle of the perturbation validation based on experimental exploitation of so-called 'physical type' experiments. Indeed, in the series of these 47 performed experiments, many are related to the same geometries with the same FP. They exactly have the same number of rods in the driver array.

Thus, for two different solutions FP1 and FP2 of the same FP, by using the critical heights difference $H_{c2} - H_{c1} = \Delta H_c$, one can obtain ΔKeff knowing the value δK/δH at H_{c1}:

$$\Delta K = (\delta K/\delta H)_{Hc1} \times \Delta H_c \quad (4)$$

δK/δH is obtained by deriving the representative function Keff, K = F(H). This latter one is determined by mathematical fit on independent MORET 4 keff calculations (with standard deviation = 33.10^{-5}) of the benchmark for various array water heights. For H, one obtains:

$$(\delta K/\delta H)_H = [\delta F(H)/\delta H]_H \quad (5)$$

Thus, the derivation method gives:

$$\Delta K = [\delta F(H)/\delta H]_{Hc1} \times \Delta H_c \quad (6)$$

If ΔH is not too large, i.e. the tangent slope at the curve K = F(H) does not vary or slightly between H_{c1} and H_{c2}, this ΔK calculation method is correct (see Figure 3). If not, it is preferable to use the integral between H_{c1} and H_{c2}, classically giving:

$$\Delta K = I\,[\delta F(H)/\delta H]\,dH = F(H)_{Hc2} - F(H)_{Hc1} \qquad (7).$$

For example, the Figure 4 displays Keff variations of some FP experiments, against water height, performed in the same driver array 25 x 25 – 25.

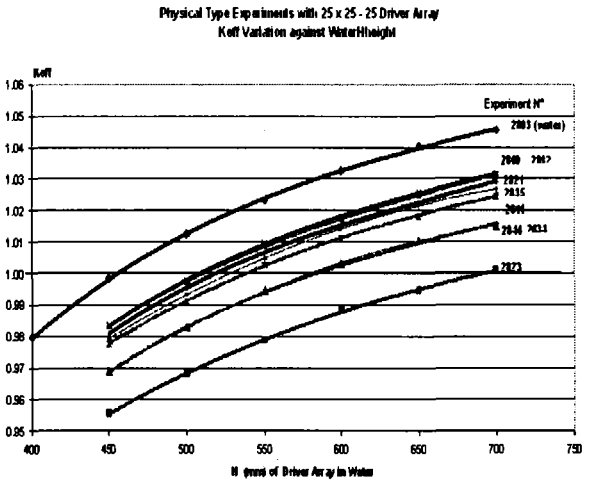

Fig. 4 Determining curves K = F(H) for the same array 25x 25 – 25 with various FP and water in the central tank.

3.3 Results and Comments

The following Table 1 presents some calculation results, based on derivation (column 4), integration (column 5) and MORET 4 'Perturbation' (column 6), against the experimental difference of critical heights ΔH (column 3). The initial (nominal) FP in column 1 is perturbed (changed) by the FP of column 2. The lowest value of correlation coefficients ρ (among the 6) obtained for each MP calculation is also given.
As can be seen, symmetric cases (for instance, cs05 changed by cs10 and cs10 changed by cs05) give results of fairly equal but with opposite values.

The Figure 5 displays these ΔK variations against ΔH when ΔH < 70 mm.

As it can be seen on Figure 5, for small variations of ΔH, the variations of ΔK against ΔH are quite linear and can be approximated by line 1, slope of which is 24.10^{-5}/mm. When ΔH increase, ΔK can be approximated by line 2, slope of which is 9.10^{-5}/mm or more precisely by a fitted curve of degree 3

Table 1 Results of Experimental Validation of MORET 4 Perturbation against FP critical Experiments

FP case		ΔH_{exp} (mm)	ΔK Calculation 10^{-5}			ρ
1	2	3	4	5	6	7
cs05	cs10	49.95	612	652	691	0.99233
cs07	cs077	103.85	509	723	745	0.99210
cs077	cs07	-103.85	-670	-762	-747	0.99511
cs09	cs11	- 29.8	-673	-660	-656	0.99548
cs09	cs12	-5.69	-135	-134	-90	0.98557
cs09	cs17	-3.85	-79	-78	-87	0.98756
cs10	cs05	-49.95	-633	-600	-701	0.99509
cs11	cs09	29.8	605	645	689	0.99282
cs11	cs17	25.98	527	558	575	0.99246
cs11	cs12	24.14	490	516	570	0.99159
cs12	cs11	-24.14	-484	-460	-568	0.99967
cs12	cs09	5.69	130	132	87	0.98332
cs12	cs17	1.84	37	37	5	0.99988
cs17	cs11	-25.98	-521	-493	-575	0.99405
cs17	cs09	3.85	77	78	79	0.98531
cs17	cs12	-1.84	-37	-37	-5	0.99990
rh34	rh35	67.1	1002	1171	1075	0.97842
rh35	rh34	-67.1	-1079	-895	-1085	0.98885

Note also the correlation coefficient values: for the very small ΔH value of 1.84 mm, ρ = 0.99990 while the corresponding ΔK values (37.10^{-5}) based on derivation or integration are larger than the MORET 4 Perturbation ΔK value (5.10^{-5}). In this case, the accuracy of the calculation made by the above relationship (6) or (7) depends on measurement uncertainty on the heights (by their differences and the height value of the calculation point), and on the uncertainty of the determination of the two expressions used K = F(H) and δF(H)/δH which derive from independent MORET 4 keff obtained with standard deviation = 33.10^{-5}. Thus, we assume that the MORET 4 Perturbation value is correct, while the other ΔK values are larger due to experimental uncertainties.

When ΔH > 2 mm (see for example the 3.85 mm case), all ΔK values agree very well and the experimental and statistical uncertainties do no longer have any effect.

By quadratic combination of measurement uncertainties on the heights difference and their reproducibility, one obtains 0.6 mm at 2σ levels.

Taking into account the slopes values δK/δH, determined to be from 9 to 24.10^{-5}/mm, one translates the measurement uncertainty into reactivity weights between 5.4 to $14.4.10^{-5}$.

One experiment (with water, instead of FP solution) was also exactly repeated. This reproduced experiment showed against the reference one a difference height ΔH = 1.87 mm. When quadratically combining this latter value with the former one of 0.6 mm, the uncertainty rises to 2 mm, giving ΔK between 18 to 48.10^{-5}.

Thus, we assume an average value of ± 20.10^{-5} of experimental methodology uncertainty for the

experimental validation of MORET 4 Perturbation. As seen by the 1.84 mm case, MORET 4 Perturbation itself is more accurate.

4. Numerical Validation

4.1 Method

Calculation results from MORET 4 Perturbation are compared with deterministic APOLLO Sn 2D code results, when applying the same variation (+ 10% of FP concentration). TRIPOLI4.2 Perturbation is also used. For Monte Carlo 3D codes, MORET 4 and TRIPOLI4.2 the same geometrical model is used. For APOLLO2 Sn, the 3D geometry is described in an equivalent 2D geometry, which gives a Keff near that obtained by Monte Carlo codes.

4.2 Results and Comments

Table 2 gives a sample results over 32 analysed Physical Type FP experiments.

Differences calculated by deterministic code APOLLO2 Sn 2D for + 10% variation of FP concentration (C) agree quite well with results for the same variation obtained by MORET 4 Perturbation, with standard deviation (σ) very small. ΔK are between 100 and 200.10^{-5} and close to each other (differences $\leq 20.10^{-5}$). Thus, with the former experiment validation, and those performed with 2000 calculation cases carried out during the CSM implementation, we have a very good confidence in the use of MORET 4 Perturbation, especially for FP experiments evaluations. On the contrary, TRIPOLI4.2 Perturbation results are larger (~ x 1.5) than APOLLO Sn 2D reference calculations and with larger σ (~ 45). These TRIPOLI4.2 results must be deeper analysed.

To complete the comparison, some calculations are also intended with MCNP Perturbation.

5. Detection of FP Concentration Variation

With all these results, it is possible to predict the detection limits of MORET 4 Perturbation, all being equal in the FP Physical Type benchmarks, related to Concentration variation of FP, or, which is practically the same, absorption cross section variation of FP. In Table 2, results of 10 % variation are simply applied by proportionality for reactivity limits of 20.10^{-5} and 5.10^{-5}, in each last column of the two half-tables. Indeed the values depend on the case and FP (nature and concentration).

They are under 2% for 20.10^{-5} and their average are respectively 1.2% and 0.3% for 20.10^{-5} and 5.10^{-5} limits.

6. Conclusion

In MORET 4 is implemented the calculation possibility of perturbation based on Correlated Sampling Method. 2000 calculations were already performed to validate numerically its use against deterministic APOLLO2 calculations. Here, results of an experimental validation are given. The principle is the exploitation of critical heights differences of close Physical Type experiments, in the same geometry and with the same nature of FP, differing in concentration and acidity.

Results prove the adequacy of MORET 4 perturbation well suited for the reactivity weights of uncertainties evaluations in FP experiments.

Moreover, the study shows that small absorption cross section variation of FP (1.2 – 0.3 %) can be detected by MORET 4 Perturbation, all being equal. TRIPOLI4.2 Perturbation results, less accurate, should be deeper analysed.

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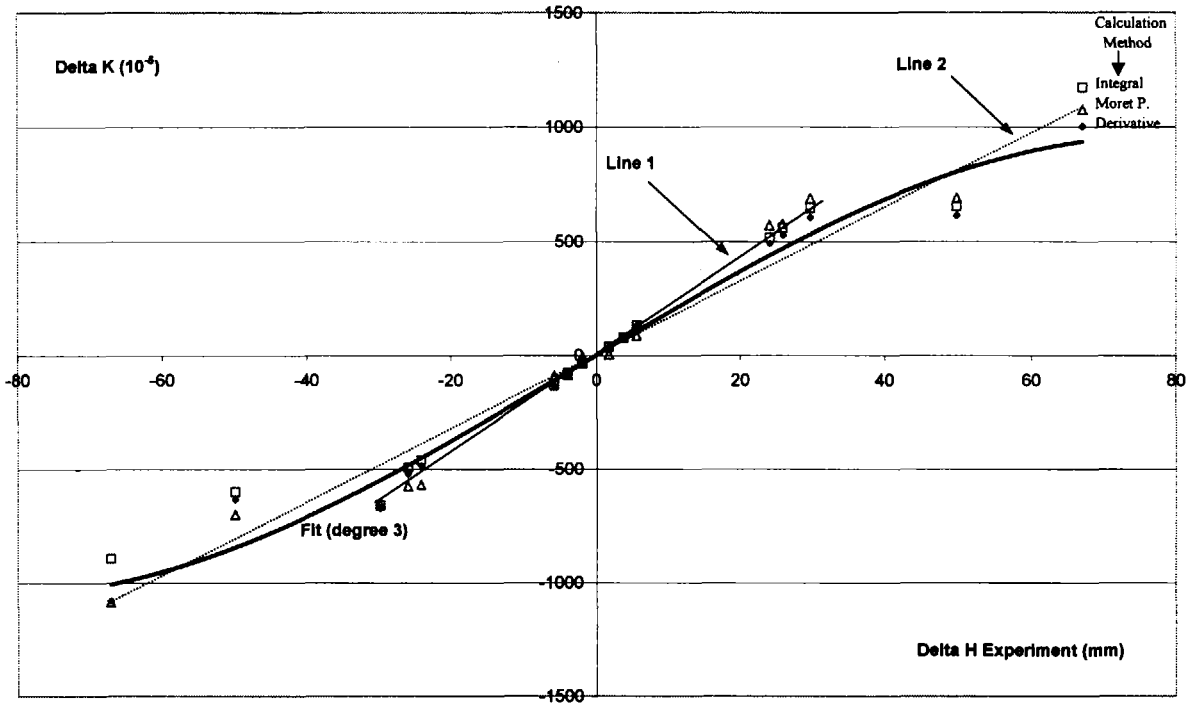

Fig. 5 Variation of various calculated ΔK against the experimental ΔH

Table 2 Numerical Validation of MORET 4 Perturbation. Detectability of Variation of FP Concentration.

	ΔK (10^{-5}) Calculations for C FP + 10%			C FP variation ↓ % for limit ↓			ΔK (10^{-5}) Calculations for C FP + 10%			C FP variation ↓ % for limit ↓	
case	MORET 4	Sn	TRIPOLI4 (σ)	20.10^{-5}	5.10^{-5}	case	MORET 4	Sn	TRIPOLI4 (σ)	20.10^{-5}	5.10^{-5}
rh33	187	189		1.07	0.214	nd22	128	131	451 (43)	1.56	0.390
rh34	178			1.12	0.280	sm23	188			1.06	0.265
rh35	129		190 (45)	1.55	0.388	sm24	186	170		1.06	0.265
rh37	147			1.36	0.340	sm25	198			1.01	0.253
cs05	148		254 (46)	1.35	0.340	sm26	183		417 (45)	1.09	0.273
cs07	158	138	221 (47)	1.27	0.318	sm27	185	198		1.09	0.273
cs11	139		238 (45)	1.44	0.36	gd28	152		387 (44)	1.32	0.330
cs077	118			1.69	0.423	gd29	159	160		1.26	0.315
cs08	122			1.64	0.410	gd30	160			1.25	0.315
cs09	105			1.90	0.475	gd31	127			1.54	0.385
cs10	111		217 (46)	1.80	0.450	gd32	125			1.60	0.400
cs12	101			1.98	0.495	mix44	173			1.16	0.290
cs17	100			2.00	0.500	mix45	191			1.05	0.263
cs18	122			1.64	0.410	mix46	190	197		1.05	0.263
nd21	112			1.79	0.448	sm47	179	184		1.12	0.280
						sm48	143		394 (45)	1.40	0.350
Average										**1.2**	**0.3**