

Impact of correlations between core configurations for the evaluation of nuclear data uncertainty propagation for reactivity

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Abstract. The precise estimation of Pearson's correlations, also called “representativity” coefficients, between core configurations is a fundamental quantity for properly assessing the nuclear data (ND) uncertainties propagation on integral parameters such as k -eff, power distributions, or reactivity coefficients. In this paper, a traditional adjoint method is used to propagate ND uncertainty on reactivity and reactivity coefficients and estimate correlations between different states of the core. We show that neglecting those correlations induces a loss of information in the final uncertainty. We also show that using approximate values of Pearson does not lead to an important error of the model. This calculation is made for reactivity at the beginning of life and can be extended to other parameters during depletion calculations.

1 Introduction

Sensitivity analysis plays an important role in the field of core physics, as nuclear data (ND) uncertainty propagation and quantification is more and more required in safety calculations of large nuclear power plant cores, as well as innovative design relevant of Gen-IV systems. An emerging need also rises for the new generation of very versatile and efficient material testing reactors (MTR), where performances and safety concern both lifetime, and isotope production. A good understanding of biases and uncertainties on reactor core calculations is essential for assessing safety features and design margins in current and future nuclear power plants, as well as in experimental reactors such as MTR. In recent years there has been an increasing demand from nuclear industry, safety and regulation for best estimate predictions to be provided with their confidence bounds.

The motivations of this work are linked to two aspects. The first one is to properly evaluate the Pearson coefficients between core states in order to make a representativity analysis, giving information to the physicists on how the reactor states are correlated in terms of uncertainties. Their knowledge allows taking into account the full part of the uncertainty. The second one is the possibility of tabulating some values of interest (uncertainties, Pearson coefficients) to correctly estimate final propagated uncertainty when direct calculations are not possible or require too important computing resources.

In this document, we will assess the impact of ND uncertainties on reactivity coefficients at the beginning of life to simplify the problem. The method can be extended to depletion calculations and to other local parameters. In this case, sensitivities can be computed with direct perturbation methods as it is done in [1]. Then, an important quantity of Pearson coefficients can be calculated for each local quantity of interest with the second equality of equation (4). For the sake of clarity, only Pearson coefficients for reactivity are analysed in this paper.

Pearson correlations are usually used in the ND covariance matrices through covariance terms between nuclear energy groups and nuclear reactions of a particular isotope. They come either from “expert judgment”, and now more and more from rigorous re-assimilation approaches used during the data evaluation. When ND uncertainties are propagated on reactor neutronics quantities, the problem of covariances between different reactor states arises. The covariances between different reactor states impact the result of the ND uncertainty propagation on neutronics parameters. The construction of adequate Pearson's representativity coefficients then enable to generate covariance between two core states, hence being ND dependent. In this paper, we show that those correlations are far from being negligible and so, Pearson coefficients have to be taken into account.

To illustrate the performances of the methodology, a material testing reactor benchmark (MTR type) 2D core benchmark has been designed, based on U_3Si_2Al fuel plate assemblies. The calculation schemes and ND library, as well as ND covariance matrices will be described. The benchmark description will be given, followed by the detailed theoretical

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analysis of the method. The last part will detail the results obtained and will give some elements of physical analysis, as well as awaited development perspectives.

2 Theory of uncertainty propagation for reactivity coefficients

The propagation law of uncertainty comes from a limited development of the calculation code functional, and is known as the ‘‘sandwich rule’’. Under a matrix form, it can be written as, for reactivity ρ :

$$\varepsilon^2(\rho) = [\underline{S}^{\rho}]^T \underline{M} [\underline{S}^{\rho}], \quad (1)$$

where $\varepsilon(\rho)$ is the standard deviation of ρ coming from the ND covariance matrix \underline{M} . $[\underline{S}^{\rho}]$ is the sensitivity vector of ρ to the ND. Knowing \underline{M} from the ND evaluation files, only $[\underline{S}^{\rho}]$ needs to be evaluated.

2.1 Sensitivity evaluation

The evaluation of $[\underline{S}^{\rho}]$ is made using standard perturbation theory [2]. Sensitivities are given by adequate procedures implemented in the APOLLO2 lattice code [3]. The most usual sensitivity value calculated by standard perturbation theory is the following:

$$\frac{\partial \rho}{\partial \sigma_k} = -\sigma_k \frac{\langle \varphi^\dagger, [\partial D / \partial \sigma_k - \lambda (\partial P / \partial \sigma_k)] \varphi \rangle}{\langle \varphi^\dagger, P \varphi \rangle} \times 10^5, \quad (2)$$

where φ^\dagger is the adjoint flux, σ_k is the k th cross-section in the order of the \underline{M} matrix, D , P and $\lambda = (10^5 - \rho) / 10^5$ are respectively disappearance, production and eigenvalue of the Boltzmann equation and $\langle \cdot, \cdot \rangle$ represents the dot product on the phase space, defined as follows:

$$\langle \varphi_1, \varphi_2 \rangle = \int_V d^3r \int_0^\infty dE \int_{4\pi} d^2\Omega \varphi_1(r, E, \Omega) \varphi_2(r, E, \Omega).$$

The calculation of sensitivities of reactivity coefficients is made using the equivalent generalized perturbation theory [4,5]. These reactivity coefficients may be linked to insertion of soluble boron or absorbing material, as well as temperature variation. The derivative of a reactivity coefficient can be expressed as a sum of reactivity derivatives. The sensitivity to a reactivity coefficient is then given by:

$$\frac{\partial \Delta \rho}{\partial \sigma_k} = \frac{\partial \rho_2 - \partial \rho_1}{\partial \sigma_k}. \quad (3)$$

The $[\underline{S}^{\rho_2}] - [\underline{S}^{\rho_1}] = [\underline{S}^{\Delta \rho}]$ vector is then built.

2.2 Evaluation of the Pearson correlation coefficients

The Pearson correlation coefficient [6] gives a formal information about the linear relation between two variables X_1 and X_2 . Its variation domain is the interval $[-1, 1]$. When X_1 and X_2 are strongly positively correlated, the Pearson $r_{X_1 X_2} \approx 1$. When they are strongly negatively correlated, $r_{X_1 X_2} \approx -1$. This value is close to 0 when the variables are uncorrelated (i.e. there is no *linear* relation between X_1 and X_2).

The Pearson coefficient can be expressed through the following relations:

$$\begin{aligned} r_{X_1 X_2} &= \frac{COV_{X_1 X_2}}{\varepsilon(X_1) \varepsilon(X_2)} = \frac{[\underline{S}^{X_1}]^T \underline{M} [\underline{S}^{X_2}]}{\sqrt{[\underline{S}^{X_1}]^T \underline{M} [\underline{S}^{X_1}] \cdot [\underline{S}^{X_2}]^T \underline{M} [\underline{S}^{X_2}]}} \\ &= \frac{\sum_i ((X_{1,i} - \bar{X}_1)(X_{2,i} - \bar{X}_2))}{\sqrt{\sum_i (X_{2,i} - \bar{X}_2)^2 \cdot \sum_i (X_{1,i} - \bar{X}_1)^2}} \end{aligned} \quad (4)$$

where \underline{S}^{X_1} is the sensitivity of a parameter to X_1 , $X_{1,i}$ is a realization of X_1 , \bar{X}_1 is the average of this realization and $COV_{X_1 X_2}$ represents the covariance between X_1 and X_2 .

All the Pearson expressions are equivalent. We understand that the knowledge of $r_{X_1 X_2}$ will be essential to express the covariance, knowing the uncertainties $\varepsilon(X_1)$ and $\varepsilon(X_2)$.

Remarks:

- The Pearson coefficient allows to analyze sample of bivariate data and not multivariate data.
- There is no transitivity relation for the Pearson coefficients, except particular cases [7]
- The independence between two variables implies that these variables are not correlated but the reciprocal is wrong. Two variables can have null Pearson coefficient while being dependent.

2.3 General theory of uncertainty accumulation

The general theory of uncertainty propagation used in this paper is described in [8].

Let's extend the propagation law to a series of perturbations which are changing the core configuration. Consider the following relation for the reactivity (Eq. (5)). In the following paragraph, we will use the configuration transformation resumed in Figure 1 as an applicative example.

We would like to determine the final reactivity ρ after having added soluble boron in the moderator, followed by a temperature increase, starting from a known reference reactivity state ρ_0 .

We can express the final reactivity state as:

$$\rho = \rho_0 + \underbrace{(\rho_1 - \rho_0)}_{\text{boron addition}} + \underbrace{(\rho_2 - \rho_1)}_{\text{temperature increase}} = \rho_0 + \Delta \rho_{\text{boron}} + \Delta \rho_{\text{temp}}. \quad (5)$$

The global propagated uncertainty corresponding to this sum (ρ) cannot be associated to the quadratic sum of the different uncertainties only, as correlations exist between the three terms of equation (5). Let's write the uncertainty to ρ as:

$$\begin{aligned} \varepsilon^2(\rho) &= [\varepsilon^2(\rho_0) + \varepsilon^2(\Delta \rho_{\text{boron}}) + \varepsilon^2(\Delta \rho_{\text{temp}})] \\ &+ [2\varepsilon(\rho_0)\varepsilon(\Delta \rho_{\text{boron}})r(\rho_0, \Delta \rho_{\text{boron}}) \\ &+ 2\varepsilon(\rho_0)\varepsilon(\Delta \rho_{\text{temp}})r(\rho_0, \Delta \rho_{\text{temp}})] \\ &+ [2\varepsilon(\Delta \rho_{\text{boron}})\varepsilon(\Delta \rho_{\text{temp}})r(\Delta \rho_{\text{boron}}, \Delta \rho_{\text{temp}})]. \end{aligned} \quad (6)$$

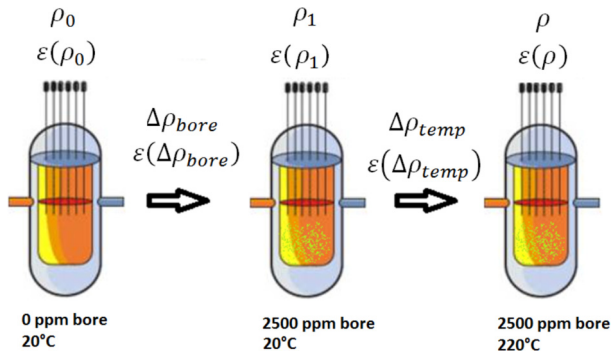


Fig. 1. Steps of uncertainties accumulations.

The first line corresponds to the quadratic sum only. The second line represents the covariances between the initial state ρ_0 and the different reactivity coefficients leading to the final state ρ_2 . The last line corresponds to the covariance between those reactivity coefficients.

Equation (6) can be written in a more convenient manner in a matrix form:

$$\varepsilon^2(\rho) = \underline{Z}^T \underline{\Omega} \underline{Z} \quad (7)$$

where $\underline{Z} = [\varepsilon(\rho_0) \quad \varepsilon(\Delta\rho_{\text{boron}}) \quad \varepsilon(\Delta\rho_{\text{temp}})]$

and

$$\underline{\Omega} = \begin{bmatrix} 1 & r(\rho_0, \Delta\rho_{\text{boron}}) & r(\rho_0, \Delta\rho_{\text{temp}}) \\ r(\rho_0, \Delta\rho_{\text{boron}}) & 1 & r(\Delta\rho_{\text{boron}}, \Delta\rho_{\text{temp}}) \\ r(\rho_0, \Delta\rho_{\text{temp}}) & r(\Delta\rho_{\text{boron}}, \Delta\rho_{\text{temp}}) & 1 \end{bmatrix}.$$

We will apply these concepts to a benchmark, in order to point out the different terms appearing in equation (6).

3 Benchmarking

3.1 Benchmark description

The 2D benchmark used in the present study is a MTR based on $\text{U}_3\text{Si}_2\text{Al}$ at 19.95% of ^{235}U fuel. A radial view is reproduced in Figure 2. A single type of assembly has been modelled to build the whole core. For the sake of simplicity, no absorbing material or control element has been included in the benchmark, the goal being only to study the propagation of ND uncertainties as one operating parameter is changed at a time: temperature, or soluble boron.

Each fuel assembly is made of 22 Zircalloy plates (in green) with a thickness of 0.13 cm. Each plate contains a fuel blade of 50 μm thickness. The blue elements represent the surrounding light water (boronless at initial reactivity stage).

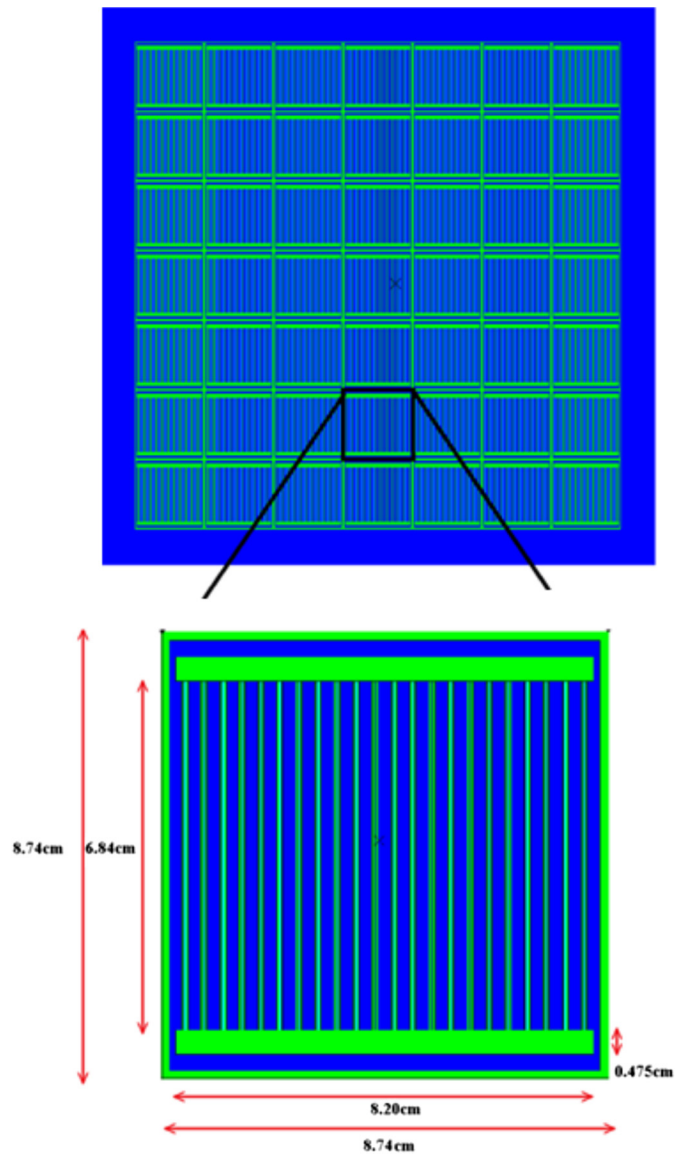


Fig. 2. Geometric representation of the benchmark.

3.2 Calculations tools

The study is made in 15 energy groups with the APOLLO2.8.3 [3] deterministic lattice calculation code on a 2D quarter of core using TDT-MOC (method of characteristics) scheme, described in [9] and *ad hoc* symmetries.

3.3 Nuclear data library and covariance data

Global uncertainties on core parameters are assessed with the propagation of ND uncertainties only. To obtain reliable covariances associated with JEFF3.1.1 evaluations [10] a ND re-estimation of the major isotopes was performed thanks to selected targeted integral experiments [11]. The CONRAD code is used to produce covariance matrices from marginalization technique [12]. This work led to the establishment of a new set of covariance matrices linked to JEFF3.1.1, called the COMAC file (COVariance MATrices Cadarache) [13]. In this covariance file, a

Table 1. Reactivity uncertainty as a function of the soluble boron concentration (pcm at 1σ).

ppm B	Temp. 20 °C					
	0	300	600	2000	2500	2800
U235	268	280	291	344	363	374
U238	60	62	65	78	83	86
H ₂ O	180	177	177	182	185	186
Al27	121	121	121	121	121	121
B10	0	14	28	90	112	124
Tot. Unc.	350	358	368	425	447	460

Table 2. Reactivity uncertainty as a function of the core temperature (pcm at 1σ).

T°C	Boron 0 ppm					
	20	100	150	180	220	250
U235	268	260	262	264	267	270
U238	60	58	61	63	66	69
H ₂ O	180	190	190	190	191	192
Al27	121	124	126	127	130	132
B10	0	0	0	0	0	0
Tot. Unc.	350	350	353	355	359	363

particular attention was paid to the re-evaluation of important isotopes ²³⁵U [14], ⁵⁶Fe [15], ²³⁸U and ²³⁹Pu [16] meanwhile other evaluations are mainly based on ENDF/B-VII covariance file.

4 Results for a “school case”

In this paragraph, we will first study what happens to reactivity uncertainty when boron is added, or when the core temperature increases. In a second part, the uncertainty on each corresponding reactivity coefficient is calculated, as well as the Pearson coefficients between these different configurations. Finally, we present an example of results obtained with and without taking into account the Pearson coefficients and we give some arguments about the possibility of tabulating these coefficients in the calculation form.

4.1 Uncertainties on reactivity

In this part, the uncertainties are calculated using the standard perturbation theory (Eq. (2)).

The uncertainties for each isotope are given by equation (1), transformed as explained in equation (8) to compute discretized sensitivities by isotope.

$$\varepsilon^2(\rho, i) = [\underline{S}^\rho(i)]^T \underline{M}(i) [\underline{S}^\rho(i)], \quad (8)$$

where i is the i th isotope, $\underline{S}^\rho(i) = (\partial\rho/\partial\sigma_{k,i})$ the sensitivity vector of reactivity to isotope i ND and $\underline{M}(i)$ the covariance matrix of ND described in the same order than $\underline{S}^\rho(i)$.

The calculated uncertainties on initial state reactivity (largely supercritical) give a result of 350 pcm at 1σ (first column of Tabs. 1 and 2). The main contributors are fission of ²³⁵U, and scattering of H₂O and ²⁷Al. In Table 1, the soluble boron concentration is increased stepwise from 0 to 2800 ppm (parts per million 10^{-6}). We observe an increase of the whole uncertainties except for ²⁷Al which remains almost constant on the whole boron range. The uncertainty increase is a linear function of the boron concentration, essentially due to the spectrum hardening caused by ¹⁰B thermal absorption. A part of the sensitivity profiles moves to higher energies, where associated uncertainties in both ²³⁵U fission, and ²³⁸U resonant capture, are also higher (Fig. 3). We observe in this figure that sensitivities are increasing after 10E-04 MeV. Particularly, for U5 capture, there is a decrease in the lower energy group whereas there is an increase in this group for fission.

At 2800 ppm, the reactivity uncertainty gets the value of 460 pcm at 1σ . For H₂O (in fact bounded hydrogen in H₂O), we observe, in the interval [0–600] ppm a slight decrease of the uncertainties, followed by an increase after 600 ppm. However, the trend remains non-significant.

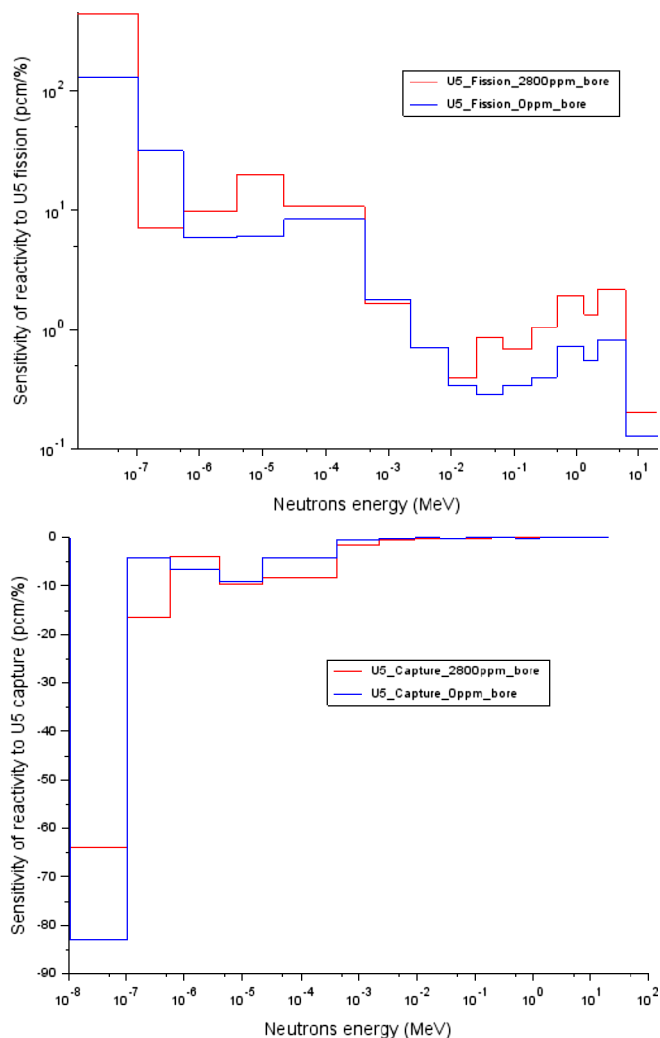


Fig. 3. Sensitivity profiles of reactivity for U5 fission capture at 0 and 2800 ppm of bore (15 groups).

Table 2 shows the variations of reactivity uncertainties when the core temperature is modified. No particular crystalline effect is taken into account for the Doppler resonant treatment. Moreover, all materials are increased to the same temperature, and no additional temperature gradient is modeled in the fuel. Uncertainty modifications are much lower compared to the boron effect. Going from 20 °C to 250 °C, the reactivity uncertainty increases from 350 to 363 pcm at 1σ , which is totally negligible. For the uranium isotopes, we observe a decrease of their propagated uncertainties between 20 and 100 °C and these uncertainties increase afterward. Globally, for the other isotopes, the uncertainties increase as the temperature rises.

The Pearson evaluation is not needed if the sensitivity calculation is possible for each core state. Performing uncertainties calculations for each state of the core needs a lot of computing resources. Establishing a database containing the main uncertainties and tabulated values of Pearson correlations could help overcome the use of important calculation resources. Indeed, the uncertainty knowledge of a particular reactor state can be interpolated

without losing too much information, as we will show below, knowing these tabulated parameters. Furthermore, the Pearson correlations, which represent physical information, give information about how the parameters are linked.

Table 3 presents results for simultaneous boron and temperature modifications. We focused on 2 temperatures. At 150 °C, the boron produces a slightly more important uncertainty on the reactivity than at 220 °C. This table explains how the uncertainties are modified by reactivity changes (cf. Sects. 4.2 and 4.3). The reactor states presented in Table 3 will be used as references for the next results.

To summarize, when the temperature decreases with an increase of the boron amount, the reactivity uncertainty coming from boron increases but the reactivity uncertainty coming from other isotopes decreases. It follows a slight decrease of the cumulated total reactivity uncertainty, mainly because, according to Table 3, the temperature impact on reactivity uncertainty is light.

4.2 Uncertainties on reactivity coefficients

Uncertainties of reactivity coefficients are calculated using equivalent generalized perturbation theory (Eq. (3)). In Table 4, we fixed the temperature and made boron variations. The $\Delta\rho$ line is the value of the reactivity coefficient and the Tot. Unc. Line corresponds to its uncertainty. We see that the reactivity coefficient uncertainty, for low boron adds, is more important at high temperature but is almost the same for the highest boron concentration (2500 ppm). The propagated value rises to 177 pcm at 220 °C for 169 pcm at 20 °C. For both temperatures, the total uncertainty value is a linear function of $\Delta\rho$ (Pearson > 0.999³). However, the function coefficients are not the same for both temperatures. Hence it is possible to predict the uncertainty value knowing the $\Delta\rho$ for boron concentration in the interval [0–2500] ppm. Moreover, the relative uncertainty of this reactivity coefficient is constant.

The trend is similar for temperature coefficients (Tab. 5). The relative uncertainty of the reactivity coefficient seems to be constant for low and high boron concentrations. The uncertainties remain weak for temperature coefficients despite the important $\Delta\rho$ when the boron concentration is low. For all the cases, the uncertainties coming from the different isotopes remain close to each other, as the uncertainties coming from boron obviously change.

These reactivity coefficient uncertainties will be used in the following to calculate the uncertainty of the different core configurations.

4.3 Pearson coefficients calculation

The Pearson correlation coefficients are the last parameters to be calculated in order to properly propagate uncertainties for a particular configuration. This coefficient,

³ This Pearson indicates the intensity of the linear relation. When the Pearson value is close to 1, the linear dependency is strong (maximum).

Table 3. Reactivity uncertainty for simultaneous variations of boron concentration and core temperature (pcm at 1σ).

ppm B	Temp. 220 °C			ppm B	Temp. 150 °C		
	100	600	2500		100	600	2500
U235	283	300	363	U235	277	295	363
U238	73	78	96	U238	67	72	90
H ₂ O	177	177	187	H ₂ O	177	176	185
Al27	127	127	129	Al27	123	124	124
B10	4	26	99	B10	5	27	106
Tot. Unc.	365	380	450	Tot. Unc.	357	373	448

Table 4. Reactivity coefficients uncertainties, on the left, at 20 °C, on the right at 220 °C for boron amount variations (pcm at 1σ).

$\Delta\rho_{\text{boron}}$	Temp. 20 °C			Temp. 220 °C		
	0->100	0->600	0->2500	0->100	0->600	0->2500
$\Delta\rho_{\text{ppm B}}$						
U235	4	29	116	36	52	125
U238	1	6	28	25	29	47
H ₂ O	2	13	38	25	34	57
Al27	0	3	13	11	14	24
B10	5	28	112	4	26	99
Tot. Unc.	7	43	169	52	75	177
$\Delta\rho$	-1141	-6658	-26 493	-1008	-6012	-23 877

Table 5. Reactivity coefficients uncertainties, on the left, at 100 ppm of boron, on the right at 2500 ppm of boron for core temperature variations (pcm at 1σ).

$\Delta\rho_{\text{Temp}}$	Boron 110 ppm		$\Delta\rho_{\text{Temp}}$	Boron 2500 ppm	
	20->150	20->220		20->150	20->220
U235	5	11	U235	4	10
U238	6	12	U238	7	13
H ₂ O	10	23	H ₂ O	11	24
Al27	5	11	Al27	6	14
B10	0	0	B10	5	12
Tot. Unc.	14	30	Tot. Unc.	16	34
$\Delta\rho$	-1359	-2866	$\Delta\rho$	-163	-383

describing the linear relation between two parameters, is calculated from the second equality of equation 2.4. The obtained values are tabulated for some configurations in Table 6. The symbol “->” represents the modified value used to calculate the $\Delta\rho$. Two kinds of information are tabulated in Table 6. The one mentioned in blue, is the simple correlation between the initial reactivity and the

reactivity coefficient $r(\rho_0, \Delta\rho)$. The second information, mentioned in red, corresponds to a correlation between two reactivity coefficients $r(\Delta\rho_1, \Delta\rho_2)$.

With the blue values, we observe that the Pearson correlation follows the same behavior than the boron concentration. However the reverse trend is observed for the temperature: the Pearson decreases as the temperature rises.

Table 6. Pearson coefficients calculated between reactivity coefficients or reference reactivity and reactivity coefficients.

		r($\rho_0, \Delta\rho_{\text{boron}}$)			
		0->100	0->600	0->2500	
Constant Boron	Constant Temp	0,3186	0,36453	0,41094	
r($\rho_0, \Delta\rho_{\text{temp}}$)	20->150	0,01097	0,02524	0,03172	0,04740
	20->220	0,07628	0,10986	0,09382	0,06187
		r($\Delta\rho_{\text{temp}}, \Delta\rho_{\text{boron}}$)			r($\Delta\rho_{\text{temp}}, \Delta\rho_{\text{boron}}$)

The red values exhibit completely different trends. The Pearson coefficient increase when the boron content increases for a temperature change from 20 to 150 °C, and is inverted if the range of temperature variation goes from 20 °C to 220 °C. However, if the correlation coefficients are relatively high for the boron concentrations, they remain low to very low for other quantities.

These correlation coefficients will be used in the next part to calculate the final uncertainty after changing the temperature and the boron amount in the core.

4.4 Example of uncertainty accumulation with non-zero correlations

In this part, we will consider an example and show the importance of the correlations term to calculate the uncertainty. We will show that some simplifications can be done in the correlation matrix.

We consider the following simple case: suppose the reactivity uncertainty for a case without boron and at 20 °C (noted $\varepsilon(\rho_0)$) is known, as well as the uncertainty of the boron insertion $\varepsilon(\Delta\rho_{\text{boron}})$, the Pearson correlation between $\varepsilon(\rho_0)$ and $\varepsilon(\Delta\rho_{\text{boron}})$, written $r(\rho_0, \rho_{\Delta\rho_{\text{boron}}})$ or the Pearson correlation between $\varepsilon(\rho_0)$ and the final case with boron $\varepsilon(\rho_0 + \Delta\rho_{\text{boron}})$, written $r(\rho_0, \rho_1)$.

We want to calculate the uncertainty of the final case $\varepsilon(\rho_1)$.

Two possibilities can be used, given by the uncertainty propagation law (Eqs. (6) and (7) with only one reactor state modification), isolating the quantity of interest. The uncertainty of state ρ_1 can be written as follows:

See the equation below:

$$\begin{aligned} \varepsilon(\rho_1) &= \pm \sqrt{[\varepsilon(\rho_0)]^2 r(\rho_0, \rho_1) - [\varepsilon(\rho_0)] + [\varepsilon(\Delta\rho_{\text{boron}})]^2 + [\varepsilon(\rho_0)] r(\rho_0, \rho_1)} \\ &= \pm \sqrt{[\varepsilon(\rho_0)]^2 + [\varepsilon(\Delta\rho_{\text{boron}})]^2 + 2[\varepsilon(\rho_0)][\varepsilon(\Delta\rho_{\text{boron}})] r(\rho_0, \rho_{\Delta\rho_{\text{boron}}})} \end{aligned}$$

A numerical application can be performed, considering a boron injection of 2500 ppm. Then, using the equation (7), one gets:

$$\begin{aligned} \varepsilon(\rho_1) &= \pm \sqrt{[350]^2 + [169]^2 + 2[350][169] \times 0.41094} \\ &= 447 \text{ pcm.} \end{aligned}$$

It corresponds to the value calculated in Table 1. Performing the application without the correlation term would give:

$$\varepsilon(\rho_1) = \pm \sqrt{[350]^2 + [169]^2} = 389 \text{ pcm.}$$

The calculated uncertainty without correlation would be 389 pcm instead of 447 pcm. This represents an error of 13% on the reactivity uncertainty estimation.

Let's try to generalize the process for different reactivity coefficients and different core configurations, as presented in Figure 1.

The final calculated reactivity is given by:

$$\begin{aligned} \rho &= \rho_0 + \Delta\rho_{\text{bore}} + \Delta\rho_{\text{temp}} = 29\,264 + (-26\,493) + (-383) \\ &= 2388 \text{ pcm.} \end{aligned}$$

Using the different tables previously presented, the correlation matrix and the uncertainty vector can be built from equation (7):

$$\begin{cases} \underline{Z} = [350 & 169 & 34] \\ \underline{\underline{\Omega}} = \begin{bmatrix} 1 & 0.41094 & 0.07628 \\ 0.41094 & 1 & 0.06187 \\ 0.07628 & 0.06187 & 1 \end{bmatrix} \end{cases}$$

Then we get $\varepsilon(\rho) = 450$ pcm which corresponds exactly to the result obtained by the uncertainty calculation using standard perturbation theory (Tab. 3). The uncertainty without correlation (replacing $\underline{\underline{\Omega}}$ by the identity matrix) would give $\varepsilon(\rho) = 390$ pcm. So, even if taking into account the temperature coefficient does not change the uncertainty, we showed that for reactivity coefficients producing important uncertainties, it is necessary to take into account the correlations.

4.5 Tabulation of Pearson coefficients

The Pearson correlations have certain stability according to the configurations. We precise that:

- The second-order Pearson coefficients like $r(\Delta\rho_i, \Delta\rho_j)$ present important variations. However, their impact on the total uncertainty remains negligible because the uncertainties linked to reactivity coefficients are less important than uncertainties on a reactivity value. Then,

taking the previous example and neglecting these coefficients, we get:

$$\left\{ \begin{array}{l} \underline{Z} = [350 \quad 169 \quad 34] \\ \underline{\underline{\Omega}} = \begin{bmatrix} 1 & 0.41094 & 0.07628 \\ 0.41094 & 1 & 0 \\ 0.07628 & 0 & 1 \end{bmatrix} \end{array} \right\} \text{Then } \varepsilon(\rho) = 450 \text{ pcm}$$

The uncertainty is then conserved.

- The first-order correlations like $r(\rho_0, \Delta\rho_i)$, impact more the total uncertainty but they can be represented by a model. For example, those coming from the boron reactivity coefficient are a linear function of the boron concentration. Moreover, variations of 25% of these coefficients (using $r(\rho_0, \Delta\rho_{\text{boron}=100 \text{ ppm}}) = 0.31860$ instead of $r(\rho_0, \Delta\rho_{\text{boron}=2500 \text{ ppm}}) = 0.41094$) do not strongly affect the final uncertainty. Then we have the following system:

$$\left\{ \begin{array}{l} \underline{Z} = [350 \quad 169 \quad 34] \\ \underline{\underline{\Omega}} = \begin{bmatrix} 1 & 0.31860 & 0.07628 \\ 0.31860 & 1 & 0 \\ 0.07628 & 0 & 1 \end{bmatrix} \end{array} \right\} \text{Then } \varepsilon(\rho) = 438 \text{ pcm}$$

This gives an error of 2.5% on the final uncertainty.

- In this particular case, the temperature correlation can be neglected, hence leading to:

$$\left\{ \begin{array}{l} \underline{Z} = [350 \quad 169 \quad 34] \\ \underline{\underline{\Omega}} = \begin{bmatrix} 1 & 0.31860 & 0 \\ 0.31860 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{array} \right\} \text{Then } \varepsilon(\rho) = 436 \text{ pcm}$$

This way of calculating uncertainty from reactivity coefficients and associated correlations can be extended to other modifications in the configuration, such as, for example, the introduction of absorbing element. In this case, when new reactivity coefficients are introduced, the dimensions of both $\underline{\underline{\Omega}}$ matrix and \underline{Z} vector are increased.

In Section 2.1, we wrote that Pearson coefficients only allow analyzing samples of bivariate data. Increasing the dimensions of the $\underline{\underline{\Omega}}$ matrix and the \underline{Z} vector is not in contradiction with Section 2.1. In fact, if we consider a new perturbation of reaction state, a row and a column to the $\underline{\underline{\Omega}}$ matrix must be added. These new Pearson coefficients represent correlations between the new state of reactor taken into account, and the previous ones. The new $\underline{\underline{\Omega}}$ matrix then becomes:

$$\underline{\underline{\Omega}} = \begin{bmatrix} 1 & r(\rho_0, \Delta\rho_1) & r(\rho_0, \Delta\rho_2) & r(\rho_0, \Delta\rho_3) \\ r(\Delta\rho_1, \rho_0) & 1 & r(\Delta\rho_1, \Delta\rho_2) & r(\Delta\rho_1, \Delta\rho_3) \\ r(\Delta\rho_2, \rho_0) & r(\Delta\rho_2, \Delta\rho_1) & 1 & r(\Delta\rho_2, \Delta\rho_3) \\ r(\Delta\rho_3, \rho_0) & r(\Delta\rho_3, \Delta\rho_1) & r(\Delta\rho_3, \Delta\rho_2) & 1 \end{bmatrix},$$

where $r(\Delta\rho_i, \Delta\rho_j)$ represents the correlation coefficient between the i th and j th state modification of the reactor.

5 Conclusions

In this paper, we have detailed a particular application of ND uncertainty propagation on reactivity coefficients, and used calculated Pearson correlations coefficients to extrapolate reactivity uncertainties for different core configurations. These correlations are necessary for applying rigorous uncertainty propagation. We showed on a very simple case that they cannot be neglected, with the exception of some values of low reactivity coefficient uncertainties or of second-order correlations. The reactivity uncertainty, calculated without taking into account these correlations is underestimated by about 13% (~ 80 pcm) in our MTR benchmark.

Of course, values obtained here are case-dependent, and should be different for different benchmarks. However, correlation coefficients can be tabulated and modeled for extrapolation of reactivity uncertainties, as we showed that perturbations of these correlations do not induce important errors on the final propagated uncertainty.

The calculation of these correlations can be extended for other core parameters such as local power factors or isotopic concentrations in the case of burnup calculations. The accurate knowledge of all these uncertainties and correlations could, in the future, feed an “uncertainty data base” associated to a cumulating model, dedicated to actual MTR or nuclear power plants. This would allow an easy and direct access to ND propagated uncertainties of all local and global core parameters for any configuration.

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