Impact of Nuclear Data Uncertainties on the Reactivity Coefficients of ALFRED

N.Garcia-Herranz¹, P.Romojaro¹, G.Grasso², F.Lodi³, F.Alvarez-Velarde⁴, D.Lopez⁴

¹Universidad Politécnica de Madrid (UPM), Madrid, Spain

²Agenzia Nazionale per le Nuove Tecnologie, l'Energia e lo Sviluppo Economico Sostenibile (ENEA), Bologna, Italy

³Università di Bologna (UniBO), Bologna, Italy

⁴Centro de Investigaciones Energéticas, Medioambientales y Tecnológicas (CIEMAT), Madrid, Spain

E-mail contact of main author: nuria.garcia.herranz@upm.es

Abstract. The advancement of the design of ALFRED – the Advanced Lead-cooled Fast Reactor European Demonstrator - beyond the conceptual phase, passes through the analysis of the impact of uncertainties, notably to what concerns safety-related conditions. Focusing on the design of the core, nuclear data are the main source of uncertainties, so their evaluation is of utmost importance in order to assess the favorable behavior of the system under beyond-Design Basis transients, as resulting from previous best estimate analyses standing on nominal values of the system parameters. This work presents the results of the sensitivity/uncertainty analysis of the ALFRED core on the main reactivity effects as a basis for computing the feedback coefficients. The sensitivity analysis allowed pointing out firstly the most relevant cross sections for every response function and the key regions where safety parameters needed to be evaluated. Uncertainty analysis allowed then establishing a possible range of confidence for the reactivity effects. The adjoint-based technique involved in TSUNAMI-3D module from SCALE6 system was used. The confidence intervals identified for each reactivity effect - once combined to provide confidence intervals for the feedback coefficients - will permit transient calculations to propagate uncertainties into transient behavior, after pointing out the most unfavorable - yet physical - set of reactivity coefficients for the selected transient scenarios. This will in turn provide an exhaustive picture of the influence of nuclear data uncertainties on core performance, identifying key parameters and possibly indicating specific actions required to achieve the aimed safety performances.

Key Words: ALFRED, nuclear data, sensitivity and uncertainty analysis, reactivity coefficients.

1. Introduction

One key research goal for ALFRED is the demonstration of favorable transient behavior under accident conditions. Such behavior depends on the reactivity coefficients of the core. Those coefficients can be evaluated using accurate computational tools available nowadays; however, results will be affected by different sources of uncertainty, such as uncertainties on the engineering design, on the model, on the nuclear data, etc.

The objective of this work is to perform a sensitivity/uncertainty (S/U) analysis of the ALFRED reactor to assess the impact of nuclear data uncertainties on core reactivity (k_{eff}) and on some key elementary reactivity effects. Sensitivity analysis will allow pointing out the most relevant cross sections for every response function and the key regions where reactivity

effects need to be evaluated. Uncertainty analysis will allow establishing a possible range of values for reactivity effects.

The S/U analysis performed for the ALFRED reactor core is presented in this paper. The adjoint-based technique involved in TSUNAMI-3D module from SCALE6 system was used.

2. SCALE6 system: calculation methodology

The SCALE code system, developed at Oak Ridge National Laboratory (ORNL), "provides a comprehensive, verified and validated, user-friendly tool set for criticality safety, reactor physics, spent fuel characterization, radiation shielding, and sensitivity and uncertainty analysis. For more than 30 years, regulators, licensees, and research institutions around the world have used SCALE for safety analysis and design" [1].

SCALE is structured to provide standardized sequences simplifying the user effort required to perform complex coupled calculations. For example, KENO-VI, the Monte Carlo criticality code of SCALE system, is automatically coupled with TSUNAMI-3D, the module of SCALE in charge of performing S/U analysis.

The consolidated version SCALE6.1.3 (labelled as SCALE6.1 in this paper) was used in this work, since this version has been validated through the years and is considered to provide high-fidelity reference solutions.

The methodology applied in this work can be divided in three steps, as shown in FIG. 1.

2.1.Step 1: Criticality analysis using the Monte Carlo KENO-VI code

KENO-VI is the Monte Carlo neutron transport code of SCALE6 package. In KENO-VI, the treatment of the energy variable can be either multi-group (MG) or continuous energy (CE). Since the technique used for S/U analysis requires forward and adjoint transport calculations in MG mode, MG KENO-VI criticality calculations were performed and compared with CE KENO-VI results in order to validate the problem-dependent cross section processing prior to the transport calculations.



FIG. 1. Criticality and S/U calculation sequence followed for ALFRED analysis.

2.2.Step 2: S/U analysis of k_{eff} using the multi-group TSUNAMI-3D module

TSUNAMI-3D (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation in 3 Dimensions) is the module within the SCALE6 code system that performs S/U analysis of three-dimensional geometry systems to nuclear data. In SCALE6.1, the analysis is based on first order perturbation theory in MG, being referred as MG TSUNAMI-3D.

First, MG TSUNAMI-3D provides automated, problem-dependent cross sections, computing not only the resonance self-shielded cross sections but also their sensitivities to the input data: the implicit sensitivities. Then, two MG KENO-VI calculations are performed, one forward and one adjoint, being the explicit sensitivities computed from the product of forward and adjoint fluxes via first-order linear perturbation theory. Next, TSUNAMI-3D calls the SAMS module to compute the sensitivity coefficients, sum of the implicit and explicit components.

The complete sensitivity coefficient of k_{eff} to a single energy group of a particular nuclidereaction cross-section Σ_x is given as a relative value and indicates the relative change of the calculated k_{eff} to relative changes in Σ_x (% change in k_{eff} per 1% change in Σ_x):

$$S_{k,\Sigma_{\rm x}} = \frac{dk/k}{d\Sigma_{\rm x}/\Sigma_{\rm x}}$$

The complete sensitivity coefficient is calculated as the sum of the implicit and explicit terms:

$$S_{k,\Sigma_{x}} = (S_{k,\Sigma_{x}})_{implicit} + (S_{k,\Sigma_{x}})_{explicit}$$
:

the implicit component takes into account the change of k_{eff} due to the effect of the perturbation in the resonance shielded values of other cross sections (or energy groups):

$$\left(S_{k,\Sigma_{\rm x}} \right)_{implicit} = \sum_{reactions\,y} \frac{\partial k/k}{\partial \Sigma_{\rm y}/\Sigma_{\rm y}} \frac{\partial \Sigma_{\rm y}/\Sigma_{\rm y}}{\partial \Sigma_{\rm x}/\Sigma_{\rm x}} ;$$

the explicit component represents the effect on k_{eff} of perturbing one self-shielded cross section in the transport operator:

$$\left(S_{k,\Sigma_{\mathrm{x}}}\right)_{explicit} = \frac{\partial k/k}{\partial \Sigma_{\mathrm{x}}/\Sigma_{\mathrm{x}}}$$

The Integrated Sensitivity Coefficients (ISC) are the integral over the whole energy range of the sensitivity coefficients of one cross section.

Finally, SAMS makes use of the relative sensitivity vector S_k as well as the SCALE6 nuclear data covariance matrix $COV_{\Sigma\Sigma}$ to compute the relative uncertainty of k_{eff} (evaluated as relative standard deviation) through the "Sandwich Formula":

$$\frac{\Delta k}{k} = \sqrt{\mathbf{S}_k^T \mathcal{C} \mathcal{O} \mathbf{V}_{\Sigma \Sigma} \mathbf{S}_k} \ .$$

The covariance matrix $COV_{\Sigma\Sigma}$ contains the cross section relative covariance data evaluated for all reactions Σ (in all energy groups). That matrix is symmetric; diagonal terms are relative variances and off-diagonal terms are relative covariances. The value of the relative uncertainty in k_{eff} ($\frac{\Delta k}{k}$) is usually given in % or in pcm (10⁻⁵).

2.3.Step 3: S/U analysis of safety coefficients using TSAR module

The TSAR (Tool for Sensitivity Analysis of Reactivity Responses) module performs S/U calculations for eigenvalue-difference responses such as reactivity effects.

Given two defined states of a reactor, referred as nominal or unperturbed (1) and perturbed (2), the reactivity effect can be calculated as follows (note that $\rho_{1\rightarrow 2}$ refers to the variation of the reactivity of the unperturbed and perturbed states):

$$\rho_{1\to 2} = \rho_2 - \rho_1 = \left(1 - \frac{1}{k_2}\right) - \left(1 - \frac{1}{k_1}\right) = \frac{k_2 - k_1}{k_2 \cdot k_1}$$

If two MG TSUNAMI-3D calculations are performed, for both the nominal and perturbed states, the relative k_{eff} sensitivity coefficients to variations of the parameter Σ for both states are available:

$$S_{k1} = \frac{dk_1/k_1}{d\Sigma/\Sigma} \quad S_{k2} = \frac{dk_2/k_2}{d\Sigma/\Sigma} ;$$

then, TSAR combines the sensitivities for both states to produce sensitivities in the reactivity coefficient $\rho_{1\rightarrow 2}$:

$$S_{\rho,\Sigma} = \frac{d\rho_{1\to2}/|\rho_{1\to2}|}{d\Sigma/\Sigma} = \frac{\frac{S_{k2}}{k_2} - \frac{S_{k1}}{k_1}}{|\rho_{1\to2}|} = \frac{S_{\rho}^{absolute}}{|\rho_{1\to2}|} \ ,$$

being S_{ρ} the relative sensitivity coefficient and $S_{\rho}^{absolute}$ the absolute sensitivity coefficient.

If S_{ρ} denotes the matrix containing the relative sensitivity coefficients and $COV_{\Sigma\Sigma}$ is the SCALE covariance matrix, the uncertainty in the reactivity coefficient (evaluated as the relative standard deviation) can be calculated as follows:

$$\frac{\Delta \rho_{1 \to 2}}{\rho_{1 \to 2}} = \sqrt{\mathbf{S}_{\rho}^{T} \mathcal{C} \mathcal{O} \mathbf{V}_{\Sigma \ \Sigma} \, \mathbf{S}_{\rho}} \quad .$$

It is important to mention that TSAR defines the relative sensitivity coefficient with respect to the absolute value of the reactivity (reactivity effect can be positive or negative). In this way, the relative sensitivity gives the % change in the reactivity effect due to a change of 1% in the cross section:

- if the relative sensitivity coefficient is positive, it means that the value of the reactivity increases upon an increase of the cross section value: a positive reactivity will become more positive and a negative reactivity will become less negative;
- if the relative sensitivity coefficient is negative, it means that the value of the reactivity decreases upon an increase of the cross section value: a positive reactivity will become less positive and a negative reactivity will become more negative.

It is not straightforward to interpret the meaning of the sensitivity coefficients of the reactivity effects, since for a given change in a cross section, k_{eff} values of both the nominal and perturbed states will change, and the sensitivity coefficient will indicate the state more sensitive to that change. In consequence, a sensitivity analysis of the reactivity effect allows identifying the key quantities that can lead to biases in the reactivity response.

3. ALFRED modeling and validation of the model

A 3-D heterogeneous model for KENO-VI code has been developed for the ALFRED core configuration [2] at Beginning of Cycle (BoC) and nominal operating conditions (dilated geometry). Specifications were taken from [3]. The radial and axial layouts of the core are showed in left and right frames of *FIG. 2*.



FIG. 2. Radial (left) and axial (right) views of the KENO-VI 3D model of the ALFRED core.

Calculations were performed using the following options:

- Model of ¹/₄ of the core;
- 238 groups SCALE6 cross section library based on ENDF/B-VII.0 (v7-238). This library has been optimized for thermal system applications but was used since no optimal MG library for fast systems is available in SCALE;
- 44 groups covariance library in SCALE6.1 (44GROUPCOV). Some evaluations were also performed using the recently released 56 groups covariance library in SCALE6.2 (56GROUPCOV). This is a newer covariance library based on ENDF/B-VII.1 and previous SCALE6.1 data. Among the modified covariances: ²³⁹⁻²⁴⁰Pu nubar, ²³⁵U nubar, ¹H capture, several fission products, fission spectrum (Chi);
- Convergence levels in Monte Carlo calculations to minimize stochastic uncertainty in final values:
 - ≈ 10 pcm error in forward calculations (600 active generations, 200 skipped, 10^5 neutrons per generation)
 - ≈ 100 pcm error in adjoint calculations (30000 active generations, 600 skipped, $2 \cdot 10^5$ neutrons per generation);
- Spatial mesh of 10 cm for all material regions of the core model, together with a thirdorder spherical harmonics expansion of the angular flux.

In order to validate the ¹/₄ model of the core and MG cross section library, criticality calculations for the full core in CE were performed. Since some biases were reported by the development team when using the SCALE6.1 CE neutron data library [3], SCALE6.2beta version was used to perform CE criticality calculations. The results can be found in Table I. The following differences were obtained: 13 pcm between full core and quarter core calculations; 9 pcm between using ENDF/B-VII.0 or ENDF/B-VII.1; and about 200 pcm between MG and CE calculations.

4. Confidence interval of key reactivity effects

Reactivity effects were obtained by means of direct perturbed calculations, by comparison of perturbed states with respect to the nominal state.

Calculation	Mode	Core model	Library	k_{eff} $\pm \sigma$
SCALE6.2	CE	1/1	ENDF/B-VII.1	0.99712 ± 0.000099
SCALE6.2	CE	1/4	ENDF/B-VII.1	0.99699 ± 0.000088
SCALE6.2	CE	1/4	ENDF/B-VII.0	0.99690 ± 0.000082
SCALE6.1	MG	1/4	ENDF/B-VII.0	0.99904 ± 0.000095

TABLE I: KENO-VI CRITICALITY CALCULATIONS RESULTS FOR ALFRED.

4.1.Doppler effect

To evaluate the Doppler reactivity effect, several perturbed scenarios were considered (see Table II). For each case, the uncertainties due to nuclear data were computed using the SCALE6.1 covariance library (results in Table II). For the cladding, it can be seen that statistical uncertainties were higher than the cladding Doppler effect, and higher than uncertainties due to nuclear data. For the fuel, along with temperature variations separately for each fuel zone, calculations involving the simultaneous perturbation of both regions are performed in order to verify the additivity of the Doppler effect.

Reactivity Doppler values show:

- an effect slightly higher at inner zone, as a consequence of the lower enrichment;
- an effect for -300 K significantly higher than that for +300 K, according to its nonlinearity with temperature;
- the additivity of the Doppler effect, as the simultaneous increase of +300 K at both fuel zones leads to an overall effect of -112 ± 14 pcm, which is inside the statistical uncertainty of the sum of the separate effects over each zone under the same perturbation, evaluated as -58 47 = -105 pcm.

Case	Assumed temperature [K]			Doppler reactivity ρ	Uncertain nuclea	Doppler	
	Fuel INN	Fuel OUT	Clad	[pcm]	Δρ [pcm]	Δρ/ρ [%]	constant
FINN+300	1500	1200	700	-59 ±14	5.2 ± 1.2	9.0 ± 2.0	-259
FOUT+300	1200	1500	700	-47 ± 13	8.4 ± 1.0	17.7 ± 2.1	-211
FUEL+300	1500	1500	700	-112 ±14	10.3 ± 1.0	9.2 ± 0.9	-500
FINN-300	900	1200	700	108 ± 14	3.9 ± 1.3	3.6 ± 1.2	-375
FOUT-300	1200	900	700	99 ± 13	4.3 ± 1.3	4.4 ± 1.3	-342
FUEL-300	900	900	700	188 ± 13	6.7 ± 0.8	3.6 ± 0.4	-652
CLAD+300	1200	1200	1000	4 ± 13	6.8 ± 1.0	174 ± 25	
CLAD+500	1200	1200	1200	6 ± 14	7.0 ± 1.1	109 ± 18	

TABLE II: DOPPLER REACTIVITY AND NUCLEAR DATA UNCERTAINTIES.

Uncertainties in Doppler effects show:

- slightly higher values (both absolute and relative) for temperature increases;
- absolute values due to nuclear data are lower than ≈ 10 pcm for all the scenarios, so relative values in % become higher (up to 17.7%) when the Doppler is lower;
- simultaneous perturbation at both fuel zones leads to values similar to the those obtained when perturbing each single zone.

The main contributor to the uncertainties in all different scenarios was found to be the inelastic scattering of 238 U. Other reactions contributing to the uncertainty were the inelastic cross sections of 206 Pb and 207 Pb as well as the elastic cross sections of 16 O and 52 Cr. Concerning ISCs, the fission cross section of 239 Pu top ranks in all cases, varying between 1.0 and 1.4 $^{\%}/_{\%}$ in absolute value. Close to these values are found also the nubar and capture cross section of 239 Pu, the elastic scattering cross-section of 16 O, 56 Fe and 238 U and the inelastic scattering and capture cross sections of 238 U.

4.2.Coolant expansion effect

The coolant expansion – hence density reduction – effect is due to three concurring effects: i) increase of neutron leakage (reactivity reduction); ii) spectral hardening (reactivity increase); iii) capture reduction (reactivity increase). Several perturbed scenarios (see Table III) are considered to evaluate the effect of coolant expansion on criticality. The perturbed states are defined changing the density of the coolant by +20% and -20% from the nominal value.

Concerning the coolant expansion effects:

• above and below the active region values are negative, as leakage dominates;

Case	Assumed density[%]				Reactivity p	Uncertainties due to nuclear data		
	Fuel INN	Fuel OUT	Above	Below	[pcm]	Δρ [pcm]	Δρ/ρ [%]	
ABOVE+20	100	100	120	100	273 ± 13	5 ± 1	2.0 ± 0.3	
ABOVE–20	100	100	80	100	-321 ± 13	7 ± 1	2.2 ± 0.3	
BELOW+20	100	100	100	120	210 ± 13	4 ± 4	2.0 ± 2.1	
BELOW-20	100	100	100	80	-273 ± 13	7 ± 2	3.1 ± 0.9	
FINN+20	120	100	100	100	-173 ± 13	15 ± 1	8.6 ± 0.4	
FINN-20	80	100	100	100	193 ± 13	18 ± 1	9.5 ± 0.4	
FOUT+20	100	120	100	100	116 ± 13	10 ± 1	8.7 ± 0.5	
FOUT–20	100	80	100	100	-47 ± 14	17 ± 1	16.8 ± 0.7	
FUEL+20	120	120	100	100	56 ± 13	27 ± 1	56.4 ± 1.3	
FUEL-20	80	80	100	100	6 ± 14	34 ± 1	61.2 ± 1.2	

TABLE III: COOLANT EXPANSION REACTIVITY AND NUCLEAR DATA UNCERTAINTIES.

- in the inner fuel zone the value is positive, indicating that spectral hardening is the dominant component;
- for the whole core the effect is approximately the sum of the local effects, although additivity is not completely verified for the -20% case (as highly space-dependent coolant expansion effects occur).

Concerning uncertainties in the coolant reactivity effect:

- the smallest values (≈3%) are found when changing the coolant density above and below the active region; being leakage the dominant component, it is shown that is not very sensitive to nuclear data uncertainties;
- values as high as 18% are found when changing density in each of the active regions;
- the largest relative values are found for density variations in the whole core: coherently with the absolute values of the corresponding effect, uncertainties cannot be computed by combination of the uncertainties in the individual fuel zones, indicating again positive spatial correlations among the zones of the core.

The inelastic scattering cross section of ²³⁸U is by far the most important single contributor to all uncertainties. Relevance of lead isotopes cross sections is also found, with the inelastic scattering of ²⁰⁶Pb and ²⁰⁷Pb playing a role in density changes occurring in the active zone, while the elastic scattering of ²⁰⁸Pb is important for density changes above the core. By looking at the ISCs, it is interesting to observe that those scenarios where the leakage component is dominant are sensitive to elastic cross sections; conversely, scenarios dominated by the spectral hardening are sensitive to the inelastic cross sections.

4.3.Clad and Wrapper expansion effects

To simulate these reactivity effects, four perturbed states are considered by changing the density of the fuel cladding material and of the wrapper tube in all fuel assemblies by $\pm 20\%$ with respect to the nominal values. The reactivity effects and uncertainties due to nuclear data are presented in Table IV. Uncertainties are lower than 5.2% for clad expansion and lower than 6.5% for wrapper expansion. The analysis of the main contributors shows that capture of ⁵⁶Fe, capture and inelastic scattering of ²³⁸U and ²³⁹Pu nubar are the most important sources of uncertainty; the latter is also top scoring in terms of ISCs for all these reactivity effects.

Case	Reactivity p [pcm]		Uncertainties due to nuclear data			
			Δρ [pcm]		Δρ/ρ [%]	
CLAD+20	-406	± 12	14.3	± 0.6	3.5	± 0.1
CLAD-20	418	± 13	21.9	± 0.7	5.2	± 0.2
WRAP+20	-232	± 13	15.1	± 0.6	6.5	± 0.2
WRAP-20	242	± 13	13.3	± 0.5	5.5	± 0.2

TABLE IV: CLAD AND WRAPPER EXPANSION REACTIVITY AND NUCLEAR DATA UNCERTAINTIES.

4.4.Fuel expansion effect

To simulate this reactivity effect, the following perturbed states are defined:

- the fissile height is increased by 10%, remaining all densities to the nominal values;
- the density of the fuel is changed by $\pm 10\%$.

For this effect (Table V), relative uncertainties due to nuclear data are $\approx 1.2\%$. The main contributor – as expected – is ²³⁹Pu nubar, also showing an ISC of $\approx 0.6\%$ (absolute value); ²⁰⁸Pb elastic scattering and ⁵⁶Fe capture appear however as important contributors.

4.5.Diagrid and pads expansion effect

This reactivity effect is due to the dilation of either the lower core support plate (diagrid) or the wrapper tube at the quote where the pads – outward protrusions machined on the wrapper tube itself – are in contact, resulting in both an increase of the core radius and of the coolant volume fraction. A perturbed state where the pitch between the sub-assemblies in the core lattice is increased by 10% is defined. The reactivity effect results of -4361 ± 13 pcm. The absolute and relative uncertainties due to nuclear data are, respectively, 73.2 ± 0.4 pcm and $1.7 \pm 0.0\%$.

Due to the nature of the phenomenon, the inelastic scattering cross section of 238 U and the 239 Pu nubar are the main contributors; the latter has an ISC of 0.8 %/%. However, among the important contributors also appear 208 Pb elastic scattering and the inelastic scattering of 206 Pb and 207 Pb.

Case	Reacti	vity p	Uncertainties due to nuclear data				
	[pcm]		Δρ [pcm]		Δρ/ρ [%]		
HEIGTH+10	-2495	± 14	27.6	± 0.5	1.1	± 0.0	
DENS+10	3594	± 12	43.2	± 0.4	1.2	± 0.0	
DENS-10	-4354	± 14	51.2	± 0.4	1.2	± 0.0	

TABLE V: FUEL EXPANSION REACTIVITY AND NUCLEAR DATA UNCERTAINTIES.

TABLE VI: DIFFERENTIAL EXPANSION REACTIVITY AND NUCLEAR DATA UNCERTAINTIES.

Case	Reactivity p		Uncertainties due to nuclear data			
	լիզ		Δρ	[pcm]	Δρ/ρ	[%]
CR-SHIFT	-166	± 13	7.4	± 1.2	4.4	± 0.7
SR-SHIFT	-36	± 13	2.2	± 2.6	5.9	± 7.0

4.6.Differential expansion between core, vessel and control rods effect

To simulate this reactivity effect, two perturbed states are defined:

- control rods shifted upwards by 1 cm with respect to their reference position;
- safety rods shifted downwards by 1 cm with respect to their reference position.

Relative uncertainties (Table VI) are lower than 6% for both reactivity effects. However, for the scenario concerning the safety rods, the statistical uncertainty of the uncertainty due to nuclear data is higher than the value itself. Among the important contributors to the uncertainties, ²⁰⁶Pb inelastic scattering is found for the control rods scenario; the elastic scattering cross sections of ²⁰⁸Pb and ⁵⁷Fe can be found for the safety rods scenario.

5. Conclusions

A S/U analysis due to nuclear data has been performed for key reactivity effects of the ALFRED core using the TSUNAMI-3D module included within the SCALE6 system. It is shown that uncertainties in reactivity effects are nearly independent from the version 6.1 or 6.2 covariance evaluations, even if using the latest 6.2 covariance matrix leads to a lower uncertainty in k_{eff} .

Uncertainties lower than $\approx 18\%$ are obtained for the fuel Doppler effect; uncertainties for the cladding Doppler effect were not valid as the reactivity value is lower than statistical and nuclear data uncertainties. For the coolant expansion reactivity, uncertainties are lower than $\approx 18\%$ if the effects of the expansion at the different regions (inner and outer) are evaluated separately. A large uncertainty should be considered for the global expansion effect since there are positive spatial correlations among the zones of the core. Cladding, wrapper expansion and differential expansion of control and safety rods effects exhibit uncertainties lower than $\approx 6\%$. The lowest uncertainties, $\approx 1.7\%$, are found for fuel and diagrid expansion effects.

All these reactivity effects depend upon nuclides-reactions that are different from those affecting k_{eff} , proving that dedicated analyses are required. The results here presented are therefore recommended for use in the analysis of the ALFRED behavior in transient conditions, to stress test the confidence in the outstanding safety performances of the system should off-nominal feedback coefficients drive system dynamics.

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