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Nuclear Data Uncertainty Decomposition for SPERT-III RIA Experiments using SIMULATE-3K and SHARK-X

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Abstract – *The aim in this paper is to perform nuclear data uncertainty decomposition in order to quantify the contribution of each of the dominant nuclear data, involved in the Special Power Excursion Reactor Test III (SPERT-III) experiments, to the overall uncertainty. This is achieved with by the SHARK-X methodology, under development at PSI, for the propagation of nuclear data uncertainties in 2D lattice calculations, using CASMO5, down to 3D core transient simulations, using SIMULATE-3K. The uncertainty decomposition was carried out for six nuclear data quantities: U-235 fission, capture and nubar; and U-238 capture, elastic and inelastic scattering. The estimated uncertainties regarding both steady-state parameters such as k-eff and static reactivity worth, as well as dynamical quantities such as total power, reactivity, fuel temperature and enthalpy are presented. Uncertainty quantification results show the dominance of U-235 nubar, U-238 and U-235 capture cross sections on the overall uncertainties on k-eff and reactivity. In addition, the uncertainties in k-eff and reactivity obtained by simultaneously perturbing the six nuclear data are practically equal to those obtained by perturbing all existing nuclear data. Concerning transient, the U-238 inelastic scattering cross section is the most dominant parameter to the overall uncertainties in the time-dependent power, reactivity, maximum nodal fuel temperature and enthalpy, at all transient stages. However, it is interesting to note that, the second dominant contribution to the overall power uncertainty in the initial excursion phase is due to the U-235 nubar, while in the power reversal phase, the U-238 capture cross-section represent the second dominant contribution, and even the first during the last moments of the transient, to the overall uncertainty.*

I. INTRODUCTION

The Special Power Excursion Reactor Test III (SPERT-III) was a pressurized-water, nuclear research facility constructed specifically for experimental investigations of the reactor's kinetic behavior under initial conditions similar to those of commercial LWRs [1]. Apart from its size, the SPERT-III core was therefore designed such as to closely resemble that of a PWR and on this basis, a series of Rod Ejection Accidents (REA) tests representative of a wide range of initial and transient conditions were conducted, including cold start-up, hot start-up, hot standby, and full power.

A validation of CASMO-5 (C5)/SIMULATE-3K (S3K) against SPERT-III experiments was in recent years initiated by Studsvik ([2],[3]). On this basis, C5/S3K models for the SPERT-III core were in a first phase developed for the analysis of the cold start-up tests [2], then, in a second phase, the validation was enlarged to all other tests [3].

Recently, through a collaboration between PSI and Studsvik, a third phase has been performed in which the previous validation studies were complemented with nuclear data uncertainty quantification (UQ) [4]. In this context, the SHARK-X methodology [5], being developed at PSI, for the propagation of nuclear data uncertainties in C5 lattice calculations down to 3-D core transient simulations was applied for the analysis of one SPERT-III super-prompt critical test, Test 43, conducted at cold startup conditions. In that study, the sampling of the nuclear data was carried out by simultaneous random perturbation of 5 nuclear data quantities (fission, capture, elastic and inelastic scattering cross sections, and nubar) for a total of 160 isotopes, using the ENDF/B-VII.1 44-group covariance Matrices (CM) library [6].

The estimated uncertainties regarding both steady-state and dynamic were presented in [4]. Results showed non-negligible sensitivity upon the employed nuclear data library. Concerning transient results, overall, both total power and reactivity showed good agreement with the measurements. The time evolution of the standard deviation and skewness of the total power showed special shapes with relatively high maximum values. In addition, the uncertainties due to nuclear data in the two important safety parameters, i.e. maximum nodal fuel temperature (MNFT) and enthalpy (MNFE) were found to reach maximum value about 2% and 10%, respectively.

It should be noted that, the uncertainty quantification for the SPERT-III RIA experiments, presented in [4], was performed through simultaneous perturbation of all nuclear data and therefore the obtained uncertainties in terms of different steady-state and transient parameters are global results of the propagation of all nuclear data perturbations.

In order to assess the contribution of each of the dominant nuclear data involved in such transient to the overall uncertainties, the main goal in this research is to carry out uncertainty breakdown analysis which allows the quantification of the contribution of each of the dominant nuclear data to the overall uncertainties. The uncertainty decomposition analysis is conducted here for the following six dominant nuclear data quantities: U-235 fission, U-235 capture, U-235 nubar, U-238 elastic and inelastic scattering, and U-238 capture.

II. SPERT III E-CORE DESCRIPTION

The SPERT III E-core is a small, oxide fueled PWR, which has the general characteristics of a commercial plant (except for its size) and with no fission product inventory. The rated power is 20 MW, the rated flow 1.26 m^3/s and the design pressure and temperature are 17.33 MPa at 616 K. The E-core is composed of 4.8 % enriched UO2 fuel rods placed in stainless steel fuel assembly cans [1]. The E-core has 60 fuel assemblies (see Fig. 1).

The majority of fuel rods are contained in 48 fuel assemblies (FA) that contain 25 fuel rods (FR) in a 5×5 square array. There are 12 smaller FAs that contain 16 FRs arranged in a 4×4 square array with the same pitch as the 25-rod assemblies. Four of the 16-rod assemblies surround the centrally located transient control rod (CR) guide and the remaining eight form fuel followers of the eight E-core CRs. The poison section of the CR assemblies is constructed of stainless steel plate containing ^{10}B. The cruciform-shaped transient CR used for initiating the reactor power excursion is located at the core center. The transient CR also contains two sections. The lower absorber section is made of 1.35 wt% ^{10}B in stainless steel. The upper section is stainless steel and is normally in the core.

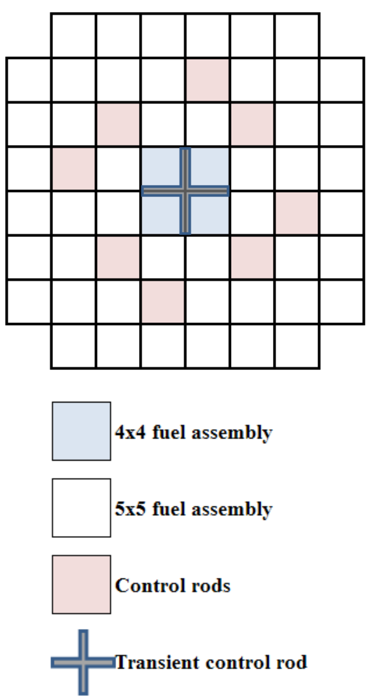

Fig. 1. Layout of the SPERT-III E-core.

The SPERT III E-core complete description can be found in reference [1], while the relevant design data for the C5/S3K simulations are provided in [2].

III. METHODOLOGY

1. CASMO-5/SIMULATE-3K Models and Code Versions

Following the conventional approach for S3K transient analyses, the two-group homogenized nuclear data (i.e. cross-sections, assembly discontinuity factors and kinetic parameters) required for the SPERT-III transient analyses are prepared via C5 2-D assembly calculations. For this, four C5 assembly models are used for each of the E-core compositions: the 5×5 FAs, the 4×4 FA surrounding the transient CR, the upper section (poison) of the CR assemblies and the lower section (fuel follower) of the CR assemblies [1]. Regarding S3K, the 3-D core model explicitly represents each of the 60 FAs. Due to the cruciform CR, the E-core is modeled as a Boiling Water Reactor (BWR) with three different fuel types: the 5×5 FA, the 4×4 FA close to the transient rod, and the CR fuel assembly with follower.

Now while the Phase-I/Phase-II validation presented in [2] and [3] were conducted based on the latest C5 code version along with the ENDF-B/VII.1 (E7.1) 586-group library, the SHARK-X methodology is currently linked to previous C5 code/library versions, i.e. V.1.07.01 version and ENDF-B/VII.0 586-group with E7r0.125.586 library. Note that the effect of the nuclear data library and CASMO-5 version has been analyzed in [4].

2. Sequence of Event and Rod Worth Adjustment

The SPERT-III tests transients were initiated by a rapid reactivity insertion via withdrawal of the transient control rod (CR) located in the central position. However, the available SPERT-III documentation does not specify the initial axial positions of the CRs but only the reactor state along with initial reactivity insertion are provided. Therefore, for the reference case, the first step of the S3K methodology is to position the eight FA with CR followers and keep the transient CR fully withdrawn in such a way to achieve a static reactivity worth matching the reported initial reactivity insertion and the second step is to find the position of the transient CR that makes the system critical. The power excursion is thereafter initiated by ejecting the transient CR, starting from a critical state. Note that for the perturbed cases, no adjustment of the CR configuration, obtained for the reference case, is introduced. However, before transient calculations are performed, SIMULATE-3K scheme for transient simulations starts by solving the steady-state neutron balance equations then the transient calculations are launched with a renormalization of the fission term in order to ensure criticality at the beginning of the transient [7].

3. SHARK-X Methodology

The SHARK-X methodology refers to a series of modules that were developed with the dedicated task to propagate nuclear data uncertainties provided in the form of covariance matrices (CM) in C5 assembly calculations [6]. Two complementary UQ approaches were in this context implemented: deterministic sensitivity and uncertainty analysis based on the direct perturbations (DP) and Stochastic Sampling (SS). The latter is used in this work and consists in sampling the nuclear data by random perturbations according to their joint probability distributions obtained from the CMs. Here, the ENDF/B-VII.1 44-group CM library for 5 nuclear data perturbations (fission, capture, elastic and inelastic scattering cross sections, and nubar) and a total of 160 isotopes are considered. It should be noted that, in the current SHARK-X version, the delayed neutron data are not perturbed and the cross sections are perturbed after the self-shielding calculations of CASMO (no implicit effect is taken into account). For each sample of the perturbed nuclear data set, a corresponding C5 calculation followed by a downstream S3K analysis is then performed. Once all n=1..N samples and associated calculations have been completed, a statistical analysis is made to estimate the first (mean), second (variance or standard deviation), and third moments (skewness) of the code output distributions. As part of this, the deviation between the estimated mean and the unperturbed reference analysis case is systematically checked and if the bias is considered as significant enough, the number of samples is increased until sufficient convergence (close to zero bias) is achieved.

IV. RESULTS

In this analysis, the simulation of the super-prompt critical test, Test 43, conducted at cold startup conditions, is carried out. Test 43 has an initial reactivity insertion of 1.21$. The experimental uncertainties in peak power and initial reactivity insertion are ±42 MW and ±0.05$, respectively. Note that the calculated reactivity is calculated by the inverse reactivity method [3].

1. Uncertainty Quantification and Decomposition Analysis

The SHARK-X calculations conducted in the current research are exactly similar to those conducted in the previous paper [4]. Hence, a Stochastic Sampling (SS) is used and consists in sampling the six dominant nuclear data quantities, i.e. U-235 fission, capture, and Nubar; U-238 capture, elastic and inelastic scattering, by random perturbations according to their probability distributions obtained from ENDF/B-VII.1 44-group CM library. For each sample of the perturbed nuclear data set, a corresponding CASMO5 calculation, using the ENDF/B-VII.0 586-group library, followed by a downstream S3K analysis is performed. Note that 300 samples were performed for each of the six nuclear data.

2. Steady-state Calculations

The steady state results in terms of k-eff and the reactivity worth are presented in Table I, Figs. 2 and 3. As it can be observed, the biases are relatively small (<30 pcm), where the maximum value is obtained for U-235 nubar (29 pcm). These give confidence in the sampling number convergence. However, for U-235 nubar, the convergence of both mean and standard deviation of k-eff is fulfilled using 300 samples, as illustrated in Fig. 2.

Table I and Fig. 3 show also the contribution of each of the 6 nuclear data quantities to the overall uncertainties in k-eff and reactivity. As it can be seen, the first three dominant contributions for both k-eff and reactivity are the U-235 nubar, U-238 Capture, and U-235 capture, respectively. U-238 elastic scattering represents the weakest contributor to the overall uncertainty.

Note also that, the uncertainty in k-eff and reactivity due to the simultaneous perturbation of the 6 dominant nuclear data (6 ND) is practically equal to that obtained by perturbing all existing nuclear data in the library (ALL ND). This means that for k-eff and reactivity, perturbing the 6 ND simultaneously represents practically the overall uncertainty.

Table I. Uncertainty Decomposition of k-eff and Reactivity.

Test 43-ENDF7.1		Ref.	Average	Bias	Std	Uncer(%)
ALL	Keff	0.99996	1.00011	15 pcm	742 pcm	0.74
	React. ($)	1.2163	1.2163	0.0000	0.0083	0.68
6 ND	Keff	0.99996	0.99977	19 pcm	741 pcm	0.74
	React. ($)	1.2163	1.2166	0.0004	0.0083	0.68
U235 nubar	Keff	0.99996	0.99967	29 pcm	583 pcm	0.58
	React. ($)	1.2163	1.2165	0.0003	0.0063	0.52
U238 CAP	Keff	0.99996	0.9998	16 pcm	272 pcm	0.27
	React. ($)	1.2163	1.2165	0.0002	0.0039	0.32
U235 CAP	Keff	0.99996	0.9998	16 pcm	178 pcm	0.18
	React. ($)	1.2163	1.2166	0.0004	0.0021	0.17
U238 ISC	Keff	0.99996	0.99995	1 pcm	142 pcm	0.14
	React. ($)	1.2163	1.2162	0.0000	0.0010	0.08
U235 FIS	Keff	0.99996	0.99998	2 pcm	96 pcm	0.10
	React. ($)	1.2163	1.2162	0.0000	0.0014	0.12
U238 ESC	Keff	0.99996	0.99996	0 pcm	1 pcm	0.00
	React. ($)	1.2163	1.2162	0.0000	0.0002	0.02

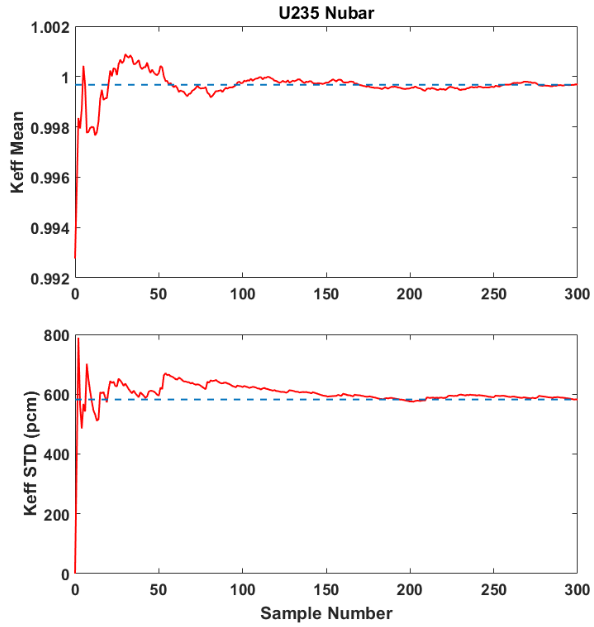

Fig. 2. k-eff Mean and STD Convergence-U-235 Nubar.

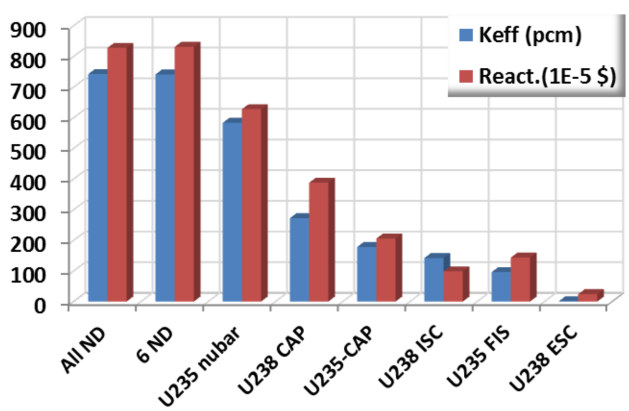

Fig. 3. Uncertainty Decomposition of k-eff and Reactivity Data.

3. Transient Calculations

In this section the transient calculations are carried out for the 6 nuclear data using SIMULATE-3K and 300 samples for each case. The duration of the transient calculation is 0.5 s using a time step of 0.3 ms in the time interval where power excursion is expected, i.e. [0.16s, 0.24s], in which temporal convergence issue may be expected due to significant variation of power. By using such small time step the temporal convergence is ensured for all samples and therefore the power response to the time step reduction is negligible. Note that, the transient CR is withdrawn from zero second with an ascending velocity and the total reactivity is completely introduced at about 0.06 s.

Fig. 4 represents the time evolution of the reactivity and the total power for the complete set of samples along with the measurement, for cases where the perturbations have been introduced to all ND, six ND, and to U-238 inelastic scattering ND, found to be the dominant contributor to the overall uncertainties in power and reactivity. The red area in the figures represents the spread of the results of the 300 samples due to the uncertainties of the perturbed nuclear data. The two dashed red curves represent the two extreme cases, within the 300 samples, corresponding to those with maximum and minimum peak power. As can be seen, when all the nuclear data are perturbed, the measured power in the initial excursion phase is well within the uncertainty area of the calculated power, while in the power reversal phase, driven mainly by Doppler feedback, the measured power is slightly outside the uncertainty area of the calculated power, however, taking into account the experimental uncertainty in power that represents about 15%[1] (error bars in blue), it can be considered that the calculated power is in good agreement with the measured one. Note that, the dashed vertical line, at about 0.21s, presented in Figures 4-8, corresponds to the time at peak power of the reference case.

Figure 5 represents the time evolution of the total power and the spread due to the separate perturbation for the additional ND, i.e. U-235 fission, U-235 capture, U-235 Nubar and U-238 capture.

Fig. 6 illustrates the time-dependent total power standard deviation, in percent, due to the perturbation of: all ND, the 6 ND, and of each of the 6 nuclear data separately. As already reported in [4], the uncertainty in power shows a double-hump shape, with a minimum value at time slightly after the time corresponding to the peak power of the reference case, and with peak values of about 16 and 12% for the case where all ND are perturbed. The reason of such shape is due to the intersection of all the curves, i.e. 300, at almost the same location, where the uncertainty become very small, e.g. equal to about 2% for the case of all ND perturbed.

As can be seen, in contrast to the steady state results, the first dominant uncertainty contribution in the transient is due to the U-238 inelastic scattering cross-section uncertainties, during the whole interval of the transient, except beyond 0.28s. This might be due to the high level of uncertainties in the U-238 inelastic scattering cross section that can reach 50%. In addition, it is interesting to note that, the second dominant contribution to the overall power uncertainty in the initial excursion phase is due to the uncertainties in the U-235 Nubar, while in the power reversal phase, the U-238 capture uncertainties represent the second dominant contribution, and even the first beyond 0.28s, to the overall uncertainty, which is somehow plausible since the U-238 capture, i.e. Doppler effect, plays

[1] It is assumed that, the experimental uncertainty in time-dependent total power is equal to that at peak power, which represents 15%, as reported in [3].

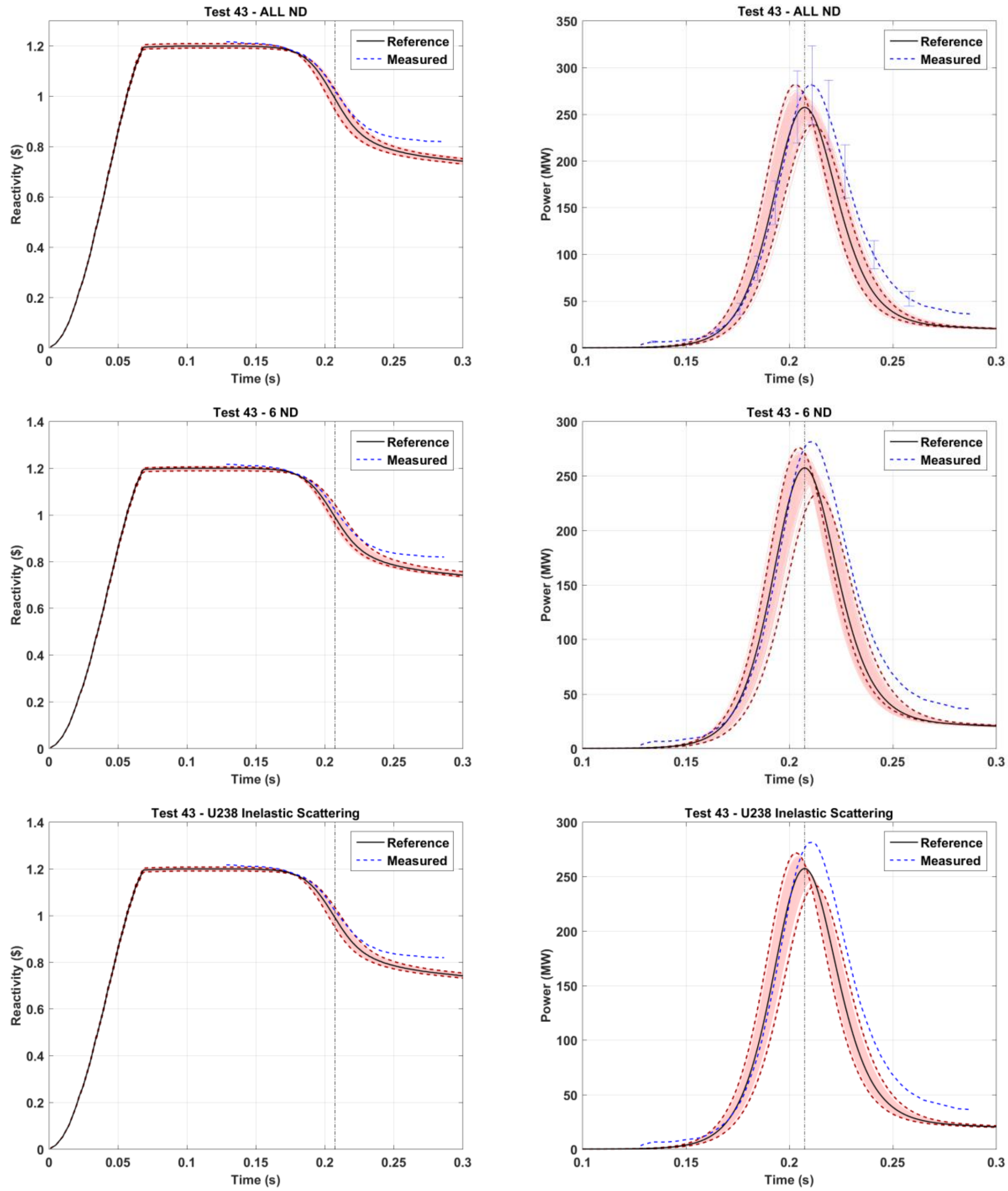

Fig. 4. Time Evolution of Reactivity and Total Power for cases with perturbation of: All ND (Top), 6 ND (Middle), Dominant ND, U-238 Inelastic Scattering (Bottom).

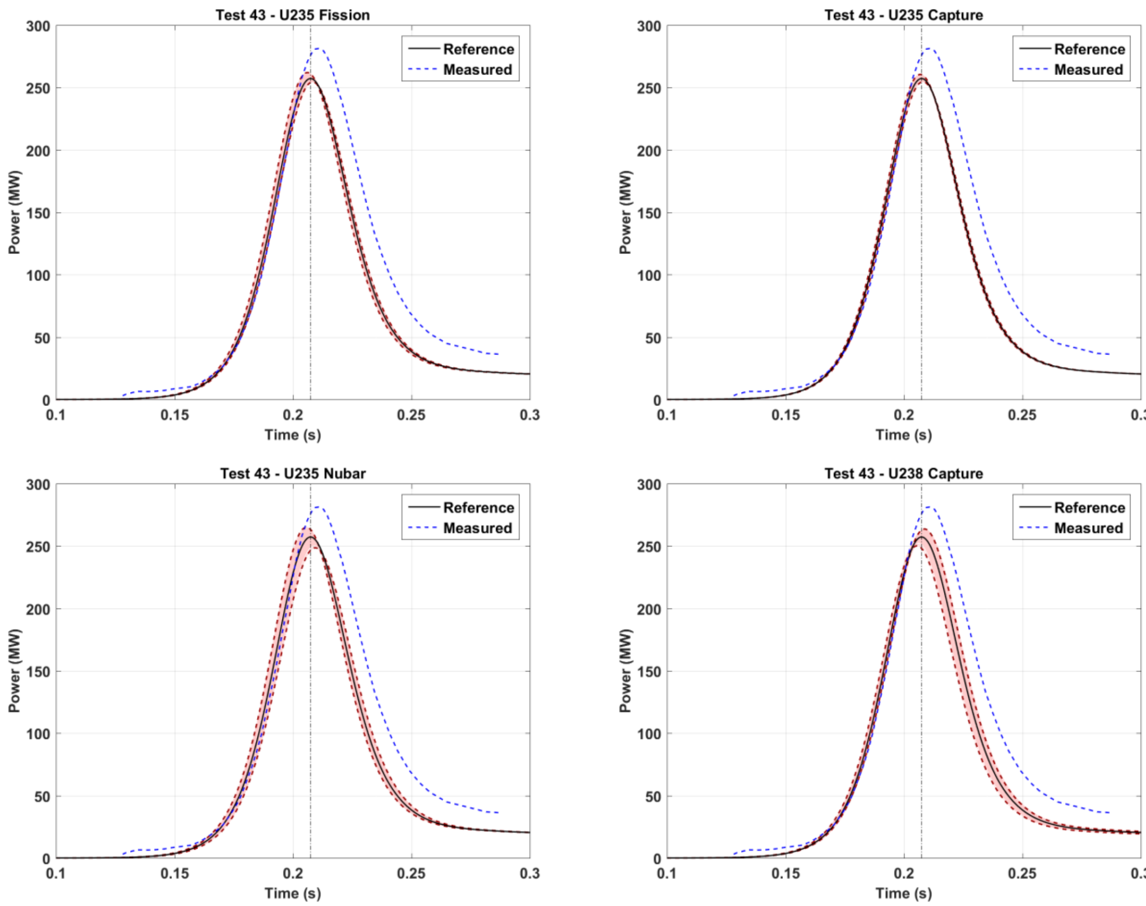

Fig. 5. Time Evolution of Total Power for cases with perturbation of: U-235 Fission (Top-left), U-235 Capture (Top-right), U-235 Nubar (Bottom-left), and U-238 Capture (Bottom-right).

the key role in the second phase of power excursion. Furthermore, it is noted that for all the cases, except for U-238 capture, the shape of the power uncertainty shows two peaks where the first one is larger.

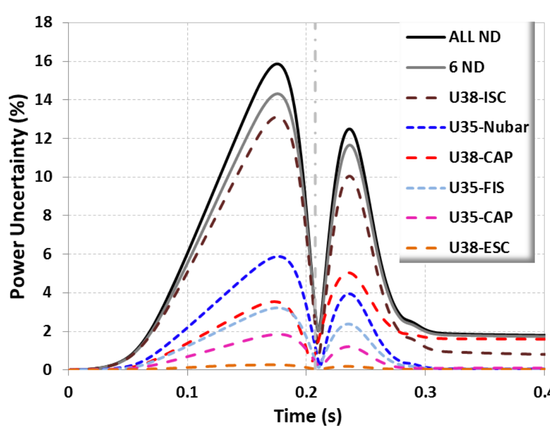

Fig. 6. Time Evolution of Relative Uncertainties in Power.

However, for U-238 capture the second peak is larger than the first, which is also expected since the Doppler effect takes place in the reversal phase of power excursion. It should be noted that the sum of the uncertainty contributions of the six nuclear data is close to the global uncertainty value, which illustrates the dominance of the six selected nuclear data. However, remaining contributions from reactions of other nuclides need to be identified, which is beyond the scope of the current research.

Figure 7 represents the time-dependent reactivity standard deviation, in percent, due to the perturbation of: all ND, the 6 ND, and of each of the 6 nuclear data separately. As can be observed the shape of the curves is similar for all cases, where the uncertainty start with almost a constant value then decreases to a minimum value at about 0.18 s, then increases to a maximum value, e.g. a peak of about 2% for the case where all ND are perturbed, and finally decreases again. Note that, the time at which the reactivity standard deviation is minimal, corresponds to the time at which the Doppler feedback starts to play the main role to reduce the total reactivity. Note also, the high values of uncertainty at around 0 s are simply because the reactivity is almost zero and any small deviation makes the uncertainty a bit large, therefore the value is not physical and should be ignored. Similar to what found for total power uncertainty, the dominant contribution to the reactivity is due to U-238 inelastic scattering, then U-235 nubar and then U-238 capture.

Figures 8 and 9 represent the time-dependent standard deviation for the maximum nodal fuel temperature, in percent, and the maximum nodal fuel enthalpy, in cal/g. as can be observed, the shape of the curves in both figures is similar. The uncertainty in temperature or enthalpy of every case, except U-238 capture, first increases to a maximum value a bit after the time of the peak power of the reference case, then deceases until around 0.26 s and finally reaches a plateau with almost constant values. However, the shape corresponding to U-238 capture is different where it increases at a first stage and reaches a peak at about the time of the peak power of the reference case, the decreases and reaches a minimum value at about 0.22 s, finally increases. Note also, that similarly to total power and reactivity, U-238 inelastic scattering and U-235 nubar represent the first and second dominant contributions to the overall uncertainty in MNFT and MNFE, respectively.

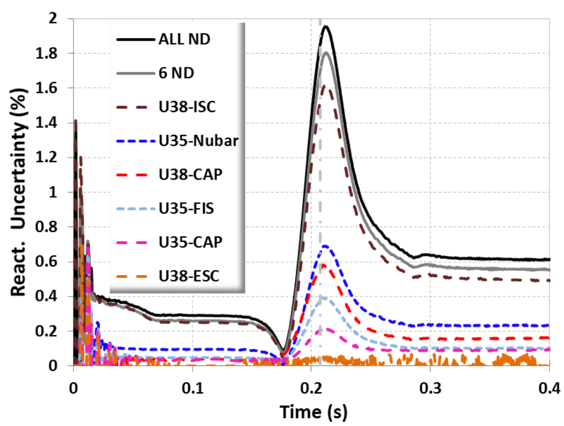

Fig. 7. Time Evolution of Relative Uncertainties in Reactivity

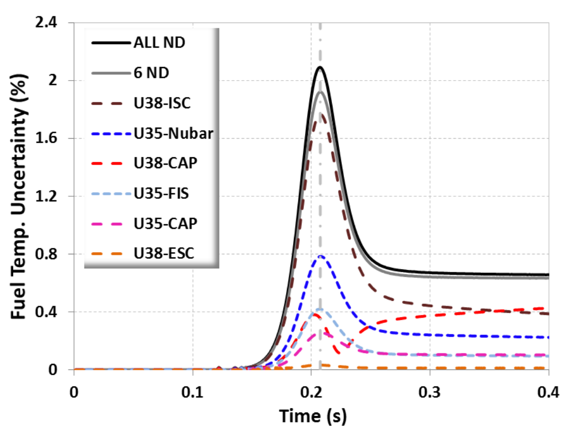

Fig. 8. Time Evolution of Relative Uncertainties in Maximum Nodal Fuel Temperature.

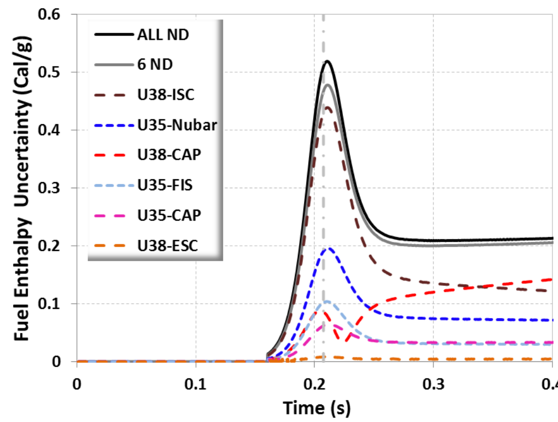

Fig. 9. Time Evolution of Relative Uncertainties in Maximum Nodal Fuel Enthalpy.

Note here that, U-238 capture represents the fourth dominant contribution to the overall uncertainty in MNFT and MNFE in the beginning of the transient, while it becomes the second dominant one beyond about 0.25 s, and even the first dominant beyond 0.33 s, which is quiet similar to what was observed for the total power, but with a time delay.

IV. CONCLUSIONS

In this paper nuclear data uncertainty decomposition has been performed in order to quantify the contribution of each of the dominant nuclear data, involved in the Special Power Excursion Reactor Test III (SPERT-III) experiments, to the overall uncertainty. This has been achieved by the SHARK-X methodology, for the propagation of nuclear data uncertainties in 2D lattice calculations, using CASMO5, down to 3D core transient simulations, using SIMULATE-3K. The uncertainty decomposition was carried out for six nuclear data quantities: U-235 fission, capture and nubar; and U-238 capture, elastic and inelastic scattering. The estimated uncertainties regarding both steady-state parameters such as k-eff and static reactivity worth, as well as dynamical quantities such as total power, reactivity, fuel temperature and enthalpy were presented. Uncertainty quantification for steady state results show the dominance of U-235 nubar, U-238 and U-235 capture cross sections on the overall uncertainty values of k-eff and reactivity. In addition, the uncertainty in k-eff and reactivity obtained by simultaneous perturbation of the six nuclear data found to be practically equal to that obtained by perturbing all existing nuclear data, which illustrates the dominance of the selected six ND. Concerning transient, the U-238 inelastic scattering represents the first dominant contribution to the overall uncertainty in the time dependent power, reactivity, maximum nodal fuel temperature and enthalpy at all transient stages, while it is interesting to note that the second dominant contribution to the overall power uncertainty in the initial excursion phase is due to the uncertainties in the U-235 nubar, while in the power reversal phase, the U-238 capture cross-section uncertainties represent the second dominant contribution, and even the first beyond 0.28s, to the overall uncertainty, which is plausible since the U-238 capture, i.e. Doppler effect, plays the key role in the second phase of power excursion.

NOMENCLATURE

ALL ND = All Nuclear Data
CAP = Capture
C5 = CASMO-5
ESC = Elastic Scattering
FIS = Fission
ISC = Inelastic Scattering
Nubar = average neutron per fission
STD = Standard Deviation
S3K = SIMULATE-3K
UQ = Uncertainty Quantification
CM = Covariance Matrix

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