VALIDATION OF SIMULATE-3K AGAINST SPERT-III RIA EXPERIMENTS WITH QUANTIFICATION OF NUCLEAR DATA UNCERTAINTIES

A. Dokhane, O. Leray, D. Rochman, H. Ferroukhi, A. Pautz
Laboratory of Reactor Physics and System Behavior
Paul Scherrer Institut, Switzerland
abdelhamid.dokhane@psi.ch

G. Grandi
Studsvik Scandpower, Inc
1070 Riverwalk Drive, Suite 150, Idaho Falls, ID, 83402, USA
Gerardo.Grandi@studsvik.com

ABSTRACT

This paper aims at integrating the quantification of nuclear data uncertainties in the validation of SIMULATE-3K against Special Power Excursion Reactor Test III (SPERT-III) experiments. To that aim, the SHARK-X methodology, under development at PSI, for the propagation of nuclear data uncertainties in CASMO5 2-D lattice calculations down to 3-D core transient simulations is applied for the analysis of a SPERT-III super-prompt critical test conducted at cold startup conditions. The estimated uncertainties regarding both steady-state parameters such as k-eff and static reactivity worth, as well as dynamical quantities such as power pulse width and enthalpies are presented. Results show non-negligible sensitivity upon the employed nuclear data library. The uncertainty quantification results show relatively small biases for k-eff and reactivity. The uncertainty in peak power is around 3%, while it is negligible for the time to peak power and the pulse width. Concerning transient results, both total power and reactivity show a good agreement with the measurements at the initial phase of power excursion, while a slightly discrepancy is obtained at the final phase of the transient. The time evolution of the standard deviation and skewness of the total power showed special shapes with relatively high maximum values. In addition, the uncertainty due to nuclear data in the two important safety parameters, i.e. maximum nodal fuel temperature and enthalpy reaches maximum value around 2% and 10%, respectively.

Key Words: **REA Analysis, SPERT-III E-core, CASMO5, SIMULATE-3K, SHARK-X, Uncertainty Quantification**

1. 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 SIMULATE-3K (S3K) against SPERT-III experiments was in recent years initiated by Studsvik ([2],[3]). On this basis, CASMO-5(C5)/S3K models for the SPERT-III core were in a first phase developed for the analysis of the cold start-up tests [2]. In a second phase [3], the validation was enlarged to all other tests. Through a collaboration between PSI and Studsvik, the objective is now to proceed with the next and third phase, namely to complement the validation with nuclear data uncertainty quantification (UQ).

At PSI, a methodology referred to as SHARK-X, is under development [4] for the propagation of nuclear data uncertainties in CASMO5 (C5) assembly calculations down to best-estimate multi-physics transient analyses using the S3K code as neutronics solver, which was designed to be a best estimate tool employing a full two-group advanced nodal method for the neutronics.

As first situation target, an UQ for the specific SPERT-III Test 43 conducted at cold start-up conditions with a super-prompt critical initial reactivity insertion of 1.21$ is presented here, noting that these results will be part of the PSI contribution to the OCED/NEA UAM Phase-II.2 benchmark [5] which includes Test 43 as part of the time-dependent neutronics benchmark cases.

2. 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 UO_2 fuel rods placed in stainless steel fuel assembly cans [1]. The E-core has 60 fuel assemblies (see Fig. 1).

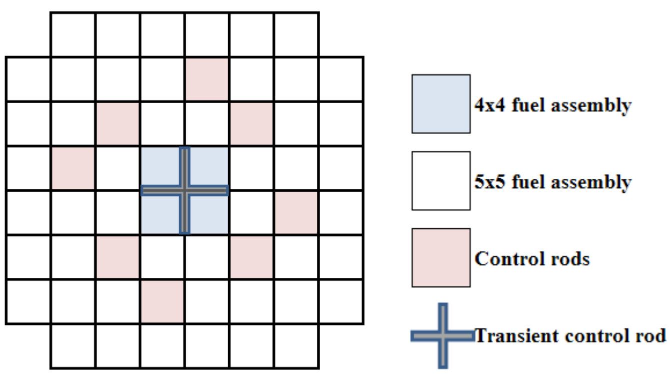

Figure 1. Layout of the SPERT-III E-core

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. 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 [1].

3. METHODOLOGY

3.1 Overview of 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 slightly older code/library versions. For this reason, the three S3K models shown in Table 2 are assessed prior to the UQ studies. S3K-3 is the original model presented in [2] and [3]. The effect of the nuclear data library can be studied by comparing models S3K-3 and S3K-2, while the effect of the CASMO-5 version can be analyzed by comparing S3K-1 and S3K-2.

Table 1. S3K Models vs. C5/Library Version

	C5	Library
S3K-1	V1.07.01	E7r0.125.586 (E7.0)
S3K-2	V2.03.00	E7r0.125.586 (E7.0)
S3K-3	V2.03.00	E7r1.201.586 (E7.1)

3.2 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 and only the reactor state along with initial reactivity insertion is provided. Therefore, the first step of the S3K methodology is to position the transient CR along with the other four CRs such as to achieve a static reactivity worth matching the reported initial reactivity insertion and preserving at the same time, core criticality at the start of the transient. The power excursion is thereafter initiated by ejecting the transient CR.

3.3 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 variance-covariance matrices (VCM) in C5 assembly calculations [4]. Two complementary UQ approaches were in this context implemented: direct perturbation (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 VCMs. Here, the ENDF/B-VII.1 44-group VCM library is employed and only 6 nuclear data perturbations (fission, capture, elastic and inelastic scattering, fission spectrum and nubar) and a total of 160 isotopes are considered. It should be noted that the delayed neutron data are not perturbed in the current SHARK-X version. 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.

4. RESULTS

4.1. Reference Case

The results of the reference case, obtained with the three distinct C5/S3K models (see Table 1), are presented in Figure 2. As can be seen, a change of code version has practically no impact on the results. On the other hand, when comparing S3K-2 and S3K-3, a significant difference is observed, noting that S3K-2 which uses E7.0 library actually provides a closer agreement to experimental data, in the initial phase of power excursion, compared to the E7.1 based S3K-3 solution, while it is the opposite situation for the final phase, i.e. power excursion (reversal). The main reason of such difference is due to the differences in the delayed neutron data between the E7.0 and E7.1 libraries. This clearly indicates a non-negligible sensitivity upon the employed nuclear data library, underlining thus the relevance of complementing the code validation with nuclear data uncertainty quantifications.

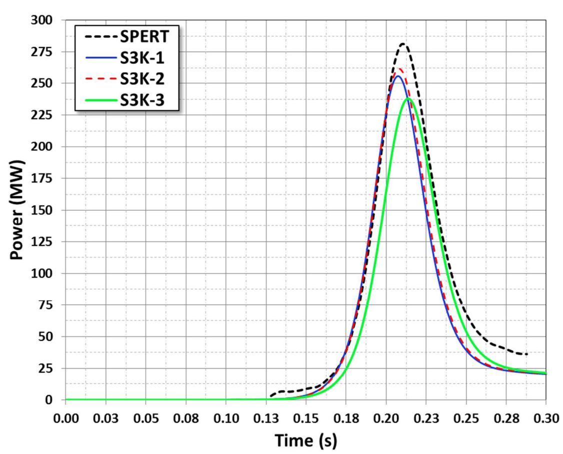

Figure 2. Test 43 Reactor Power (left) and Reactivity (right)
Comparison S3K vs. CASMO-5/Library Versions against Measurements.

4.2. UQ Analysis

Following the reference (unperturbed) case of the previous section, SHARK-X is now applied with the S3K-1 (E7.0) model, being currently the only linkable code/library version. For this purpose, 500 samples were preformed and the results in terms of selected quantities for both steady-state and transient are presented in the following sections.

4.2.1. Steady-State Calculations

The steady state results in terms of k-eff and the reactivity worth are presented in Table 2. The corresponding distribution of the k-eff values is shown on the left hand-side of Figure 3, while the right hand side presents the reactivity worth obtained for each sample along with the estimated uncertainty (1σ) range, noting that all uncertainties refer here to relative standard deviations in percent.

From these results, it can first be noted that the biases are relatively small. Regarding the k-eff uncertainty, it is close to 0.7 % which is well in line with the range of BWR and PWR eigenvalue uncertainties estimated within the OECD/NEA UAM Phase-I neutronics benchmark analyses (see e.g. [5]). Concerning the reactivity worth, the estimated uncertainty is found to be around 0.7%. Note that, although the nuclear data has been perturbed based on Gaussian-shape distribution, the distribution of k-eff and the reactivity have a non-zero skewness value, which means the existence of a certain asymmetry in the distribution.

Table 2. Uncertainty Quantification of k-eff and static reactivity worth for Test 43 with 500 samples.

	Reference	Average	Bias	Std	Uncert.(%)	Skewness
Keff	0.99996	0.99988	8 pcm	725 pcm	0.72	-0.04
Reactivity ($)	1.2163	1.2163	0.0000	0.0080	0.66	0.10

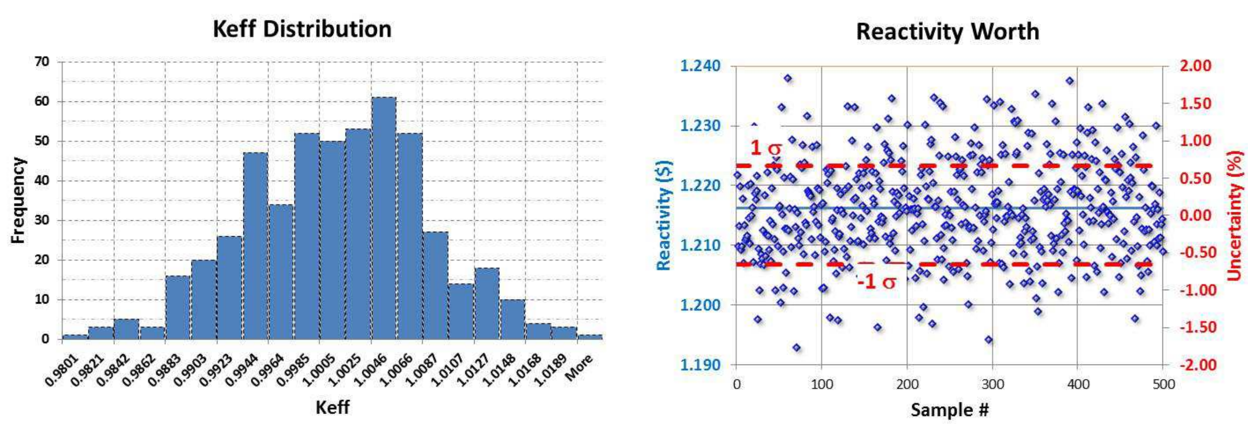

Figure 3. Distribution of k-eff (Left) and

Static Reactivity Worth Results along with Uncertainty (Right) for Test 43

4.2.1. Transient calculations

The transient calculations for 500 samples using S3K are based on the same steady-state conditions, i.e. reference case (see Section 3.2) and therefore due to the perturbation of nuclear data, the transient calculation for each sample does not necessarily start from critical core conditions and therefore the static reactivity rod worth for each sample will be different from the initial reference reactivity insertion (See Table 2). It should be noted that the transient calculations, lasting for 0.5 s, has been performed using a time step of 0.3 ms in the time interval where power excursion is expected ([0.16 s, 0.24 s]), 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.

The transient results for 500 samples in terms of power, pulse width, reactivity, maximum nodal fuel temperature and enthalpy are presented next along with their associated uncertainties.

Table 3 summarizes the statistics related to the peak power, the time to peak power, and the pulse width. As can be seen, the mean value of the total peak power is smaller than the measured one, with an uncertainty of 3%, while for the time to peak power, the mean value is almost the same as the measured value, with a standard deviation of 2 ms. For the pulse width, the mean value is similar to the measured one (around 38 ms) and the standard deviation is less than 1 ms. Part of the spread in the peak power and the time to peak power is due to the non-critical initial core conditions prior to triggering the transient for each sample and therefore a different reactivity insertion compared to the reference case, as explained in Section 4.2.1.

Table 3. Statistics of Peak power, Time to peak power and Pulse Width.

ENDF/B-VII.1 VCM	Mean	Max	Min	SDT	Uncert. (%)
Peak Power (MW)	257.3	279.2	234.9	7.6	3.0
Time to peak power (s)	0.2075	0.2125	0.2017	0.0020	1.0
Pulse width (s)	0.0382	0.0396	0.0363	0.0006	1.6

Measured Peak Power = 281.26 MW, Reference Peak Power = 257.25 MW

Figure 4 represents the time evolution of the total power, the reactivity, and the maximum nodal fuel temperature and enthalpy for the complete set of samples along with the measurements. The grey area in the figure represents the spread of the results due to nuclear data uncertainties. As can be seen, the measured power in the initial excursion phase is well within the uncertainty area of the calculated power (Top-left of Fig. 4), while in the power reversal phase, driven mainly by Doppler feedback, the measured power is clearly outside the uncertainty area of the calculated power. However, based on Figure 2 (left), if S3K-3 model, based on E7.1 library, has been used, the measured power values would be expected to be within the uncertainty range.

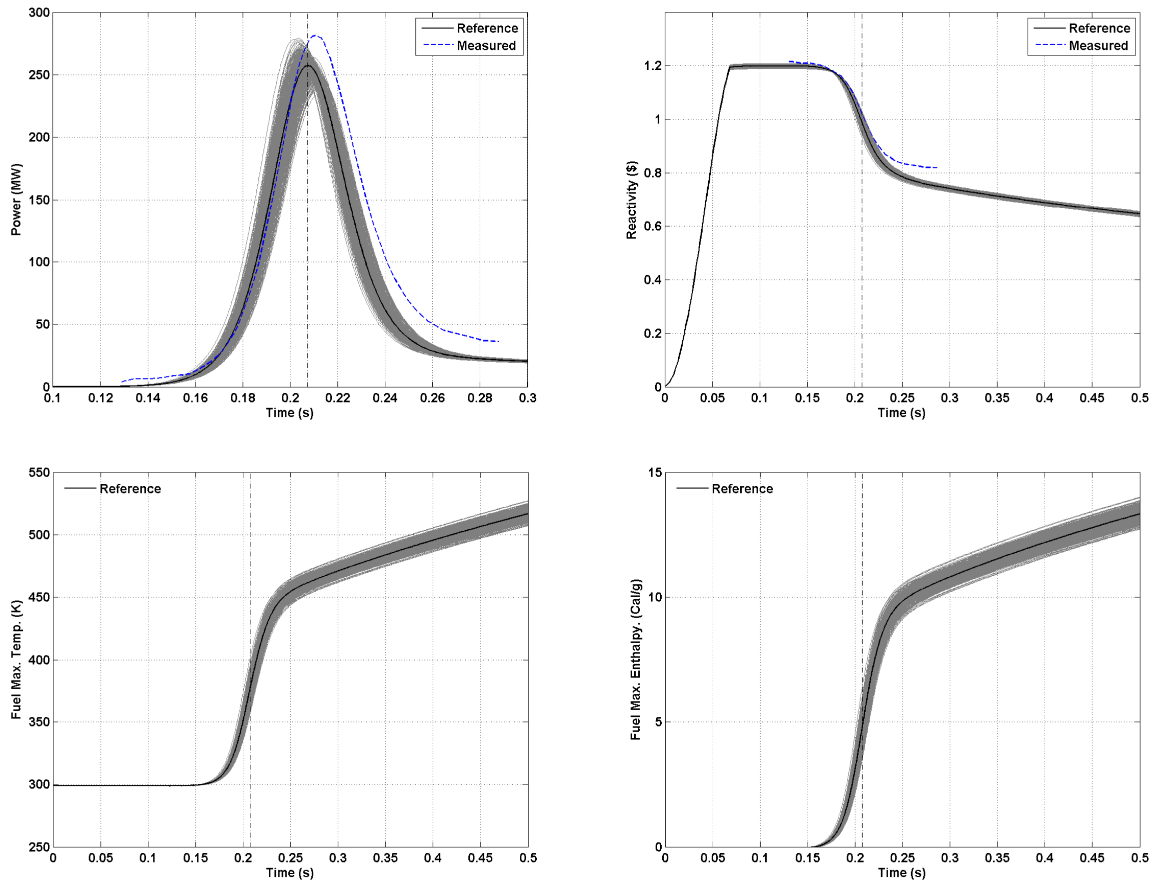

Figure 4. Time Evolution of: Total Power (Top-left), Reactivity (Top-right), Maximum Nodal Fuel Temperature (Bottom-left) and Enthalpy (Bottom-right).

Unfortunately, the SHARK-X methodology is currently based only on E7.0 library and therefore, one of the future goals is to extend SHARK-X to include E7.1 library. Another interesting observation is the obvious left shift of the peak powers of the samples compared to the reference case. This illustrates the complexity of the transient where although the perturbation of the nuclear data is based on Gaussian shape distribution (VCM), the effect on the power has a completely different distribution. Therefore, further analysis is needed to understand this issue, which is beyond the scope of the current research. Concerning the reactivity results (Top-right of Fig. 4), similarly to power results, the measured reactivity is basically within the calculated uncertainty range in the initial phase of the transient, while it is outside the uncertainty range in the transient final stage. The temporal evolution of the maximum nodal fuel temperature and enthalpy for all samples show similar shape for both quantities (bottom of Fig.4). In other words, constant value before power excursion then a sharp increase during the initial power excursion phase, finally a less sharp increase in the final phase. Note here the clear delayed effect of the power increase on the fuel temperature and enthalpy and even when the power is decreasing, the fuel temperature and enthalpy continue to increase.

The time evolution of the standard deviation for the total power, the reactivity, and the maximum nodal fuel temperature and enthalpy for the 500 samples are presented in Figure 5. As can be seen, the uncertainty in power shows a double hump (Top-left of Fig. 5), i.e. one before and one after the time where the peak power for the reference case is occurring, with peak values of around 22% and 15%, respectively. The reason for such double hump is not clear yet and further analysis is needed, which is beyond the scope of the current research. Concerning reactivity, the standard deviation reaches a maximum value of around 2% just after the time to peak power of the reference case (Top-right of Fig. 5). Concerning the maximum nodal fuel temperature and enthalpy, results show that the standard deviations along the whole transient do not exceed 8 K and 0.5 Cal/g, respectively, which correspond to relative uncertainty of 2% and 10%, respectively.

Figure 6 represents the time evolution of the skewness of the total power, quantifying the distribution asymmetry. As can be seen, the skewness is changing with time and a significant shape and sign change is observed during the power excursion with a minimal value of -0.9 at the time of the reference peak power.

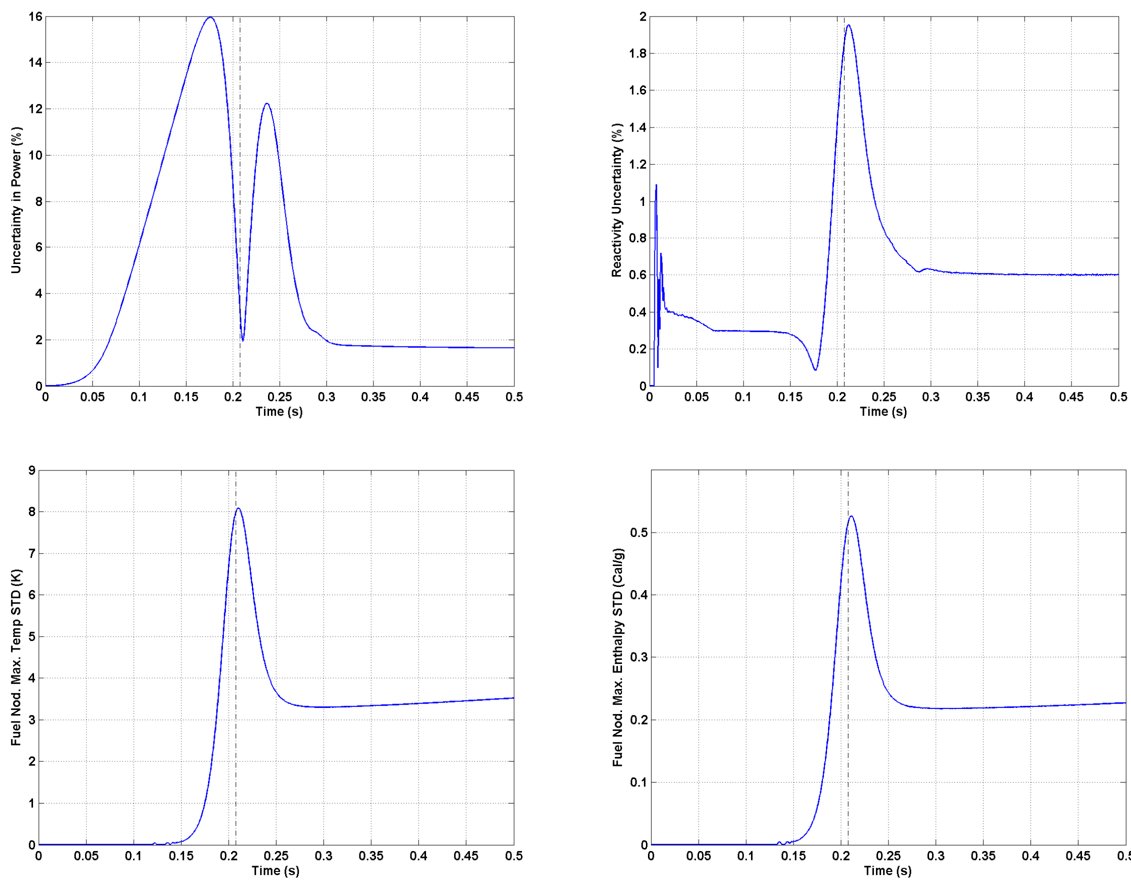

Figure 5. Time Evolution of: Relative Uncertainty for: Total Power (Top-left) and Reactivity (Top-right); Standard Deviation of Maximum Nodal Fuel Temperature (Bottom-left) and Enthalpy (Bottom-right).

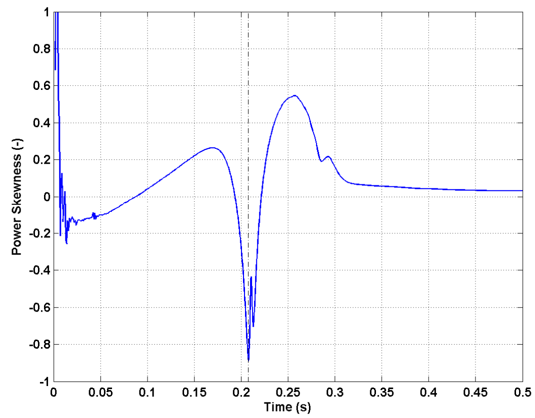

Figure 6. Time Evolution of Total Power Skewness.

5. CONCLUSIONS

The SHARK-X methodology, under development at PSI, for the propagation of nuclear data uncertainties in CASMO5 2-D lattice calculations is applied for the analysis of the Special Power Excursion Reactor Test III (SPERT-III) experiments. The main aim is to integrate the quantification of nuclear data uncertainties in the validation of SIMULATE-3K against the SPERT-III super-prompt critical test conducted at cold startup conditions. The objective is to present and discuss 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, powered pulse width and enthalpies.

The steady-state results indicated a non-negligible sensitivity upon the employed nuclear data library, underlining thus the relevance of complementing the code validation with nuclear data uncertainty quantification. Concerning the UQ, results show relatively small biases for k-eff and reactivity (around 0.7% for both quantities).

Concerning transient results, the mean value of the total peak power is found to be smaller than the measured one, with an uncertainty of 3%, while for the time to peak power, the mean value is almost the same as the measured value, with a standard deviation of 2 ms. For the power pulse width, the mean value is similar to the measured one and the standard deviation is less than 1 ms. The spread in the peak power and the time to peak power is due to the non-critical initial core conditions prior to triggering the transient for each sample and therefore a different reactivity insertion compared to the reference case. In addition, results of the time evolution of power and reactivity show a good agreement with the measurement, i.e. the measured quantities fall within the uncertainty range, in the initial phase of the power excursion, while in the final stage of the transient there is a clear discrepancy between the calculation and the measurements. However, it has been suggested that using E7.1 library instead of the E7.0 library, would significantly ameliorate the results. Furthermore, the time evolution of the second and third moments, i.e. the standard deviation and the skewness, of the total power showed special shapes and behavior which clearly illustrate the complexity of physics behind the transient. The cause of such shapes is not yet clear and therefore further analysis is need in future works. Moreover, the time evolution of the maximum nodal fuel temperature and enthalpy and their associated standard deviations have been also analyzed. Results show a clear delayed effect of the power excursion on these two quantities where the fuel temperature and enthalpy continue to increase even when the total power decreases. The uncertainty, due to nuclear data, in the two important safety parameters, i.e. maximum nodal fuel temperature and enthalpy can reach maximum values around 2% and 10%, respectively.

Uncertainty quantification and the validation of SIMULATE-3K against SPERT-III is an ongoing activity within PSI. The current results are based only on a single test, with cold start-up conditions. Therefore, in order to verify and validate the UQ with SIMULATE-3K, it is necessary to extend the current study to additional PSERT-III tests with different conditions. In addition, it is planned to extend the current study by using SCALE-6 instead of ENDF/B-VII.1 for VCM and ENDF/B-VII.1 instead of ENDF/B-VII.0 library along with CASMO5 for SHARK-X.

REFERENCES

[1] R. K. Mc. Cardell, *et al.*, "Reactivity Accident Tests Results and Analyses for the SPERT III E-core a Small Oxide-Fueled, Pressurized Water Reactor," IDO-17281, March 1969.

[2] G. Grandi and L. Moberg, "Qualification of CASMO5/SIMULATE-3K against the SPERT III E-Core Cold Start-Up Experiments", *Proc. PHYSOR 2012*, Knoxville, Tennessee, USA, April 15-20, 2012.

[3] G. Grandi, "Validation of CASMO/SIMLATE-3K using the PSERT III E-Core: Cold start-up, Hot Start-up, Hot Standby and Full Power Conditions", *Proc. PHYSOR 2014*, Kyoto, Japan, September 28-Oct. 3, October, 2014.

[4] W. Wieselquist, T. Zhu, A. Vasiliev, H. Ferroukhi, "PSI Methodologies for Nuclear Data Uncertainty Propagation with CASMO-5M and MCNPX: Results for OECD/NEA UAM Benchmark Phase I", *Science and Technology of Nuclear Installations*, Vol.(2013) Article ID 549793, 2013.

[5] OECD/NEA "Benchmark for Uncertainty Analysis in Modelling (UAM) for Design, Operation and Safety Analysis of LWRs – Volume II: Specification and Support Data for the Core Cases (Phase II)". NEA/NSC/DOC92014), Version 2.0, April 2014.