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SIMULATING FUEL BEHAVIOR UNDER TRANSIENT CONDITIONS USING FRAPTRAN AND UNCERTAINTY ANALYSIS USING DAKOTA

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ABSTRACT

Although regulatory agencies have shown a special interest in incorporating best estimate approaches in the fuel licensing process, fuel codes are currently licensed based on only the deterministic limits such as those seen in 10CRF50, and therefore, may yield unrealistic safety margins. The concept of uncertainty analysis is employed to more realistically manage this risk. In this study, uncertainties were classified into two categories: probabilistic and epistemic (owing to a lack of pre-existing knowledge in this area). Fuel rods have three sources of uncertainty: manufacturing tolerance, boundary conditions, and physical models. The first step in successfully analyzing the uncertainties involves performing a statistical analysis on the input parameters used throughout the fuel code. The response obtained from this analysis must show proportional index correlations because the uncertainties are globally propagated. The DAKOTA toolkit was used to analyze the FRAPTRAN transient fuel code. The subsequent sensitivity analyses helped in identifying the key parameters with the highest correlation indices including the peak cladding temperature and the time required for cladding failures. The uncertainty analysis was performed using an IFA-650-5 fuel rod, which was in line with the tests performed in the Halden Project in Norway. The main objectives of the Halden project included studying the ballooning and rupture processes. The results of this experiment demonstrate the accuracy and applicability of the physical models in evaluating the thermal conductivity, mechanical model, and fuel swelling formulations.

1. INTRODUCTION

The U.S. Nuclear Regulatory Commission (NRC), in 1974, formulated the first safety rules regarding nuclear reactors by creating the code of federal regulation (CFR) §50.46 with five deterministic rules having restrictive limits. The limits defined in CFR §50.46 pertained to off-normal conditions, maximum peak cladding temperature (PCT), cladding oxidation rate, and hydrogen generation. The PCT is a critical parameter in the case of transient events such as large break loss of coolant accidents (LBLOCAs). The PCT is a function of the maximum linear power of the core associated with the cooling capacity under transient conditions. These guidelines were used to define nuclear security and impose penalties for breaching the determined safety margins. However, under CFR §50.46, the deterministic safety analysis (DSA) is conducted based on an empirical method. This is problematic because the physical models currently used to simulate nuclear reactors are simplified or approximated, leading to incorrect results. The inaccuracy of the safety parameters employed in the licensing process has forced the coupling of system codes [1].

When CFR §50.46 was written, the lack of existing knowledge on nuclear performance and safety led to conservative criteria with responses based on cause and effect. In May 1989, the

NRC proposed rules for the best estimate (BE) approach. Because the BE analysis requires developing appropriate estimation techniques to determine the effects of the uncertainties, only a few practical applications were implemented using this approach. However, with the increasing interest on licensing codes applicable to LBLOCAs, the results of the probabilistic analysis replaced the precise results obtained from the BE models [2]. The development of a system using a unique code to define neutron transport codes and hydraulic systems continued during the 1990s, including a study on developing a thermal hydraulic system code (THSC) combined with the Monte Carlo code in a single computational scheme. The obtained deterministic models could be used to perform a safety analysis in the event of a nuclear accident; however, better results were obtained using either stochastic or conservative methods [3]. The transport codes based on stochastic model systems are currently used for neutron and photon transports [4].

Currently, the statistical analysis is used to extend the computational power of fuel codes in order to estimate and prove the effects of uncertainties. Nuclear systems should be evaluated using high-performance computing along with multiphysics and multiscale modeling [6]. The use of parallel computation in this process has produced new opportunities for improved multidimensional analysis. Such parallel systems can be used to determine the uncertainty propagation (UP). Under these circumstances, the best estimate plus uncertainty (BEPU) model can be used to build a more realistic result working in unison with the DSA.

2. UNCERTAINTY PROPAGATION METHODS

2.1 Uncertainty Analysis

The CFR §50.46 limits the PCT to 1204.44 °C, core-wide oxidation to under 1%, and local maximum oxidation to under 17% [7]. To model these factors in a system, uncertainty quantification (UQ) is a key step wherein the range of variation in the input parameters is defined to describe the relevant transient conditions for which the limitations were designed. The next step involves determining the UP of the system. Finally, a sensitivity analysis (SA) is conducted to validate the output results based on the levels of input dependency. Stochastic parameters may be used to assess the system of working UP models. The aforementioned BEPU approach is used to build a robust method to perform these steps based on the uncertainty analysis. The uncertainties assessed in the system simulations are determined using factors such as mechanical tolerance, boundary conditions, and physical models.

2.2 Uncertainty Methods

A nuclear power plant (NPP) system comprises 105 measured and modeled inputs and generates approximately 103 outputs. The code scaling, applicability, and uncertainty (CSAU) methodology initially used in analyzing the LBLOCA [8] served as a review basis for the emergency core cooling systems (ECCS). Specifically designed to remove residual heat from the reactor fuel rods in the event of a failure of the normal core cooling system. ECSS rules depending on the uncertainties of complex phenomena [9]. The uncertainty methodologies have undergone worldwide growth and development and are now able to generate more realistic analyses. The BEPU model can be used to compute uncertainties of stochastic and epistemic (those occurring because of a lack of knowledge) natures. Given these and other considerations, it is suggested that a framework using the BEPU analysis should be employed to replace the conservative safety assumptions [8], as the BEPU framework will help in reducing the risk in the licensing process. During the European war, studies on these methodologies were conducted and sponsored by the Organization for Economic Co-operation and Development (OECD). The BE method including the uncertainty and sensitivity evaluation (BEMUSE) is the result of the OECD-sponsored effort [10]. The BEMUSE is significant in its ability to support the SA methods applied to LBLOCA scenarios. The post-BEMUSE reflood model input uncertainty method (PREMIUM) was developed to simulate the reflood phase in a transient event [11]. These frameworks can be used to select input parameters and rank probabilities to change factors using rank correlations in the SA. A series of BEPU-LBLOCA proposals received significant collaboration from industrial vendors.

2.3 DAKOTA Toolkits

Sandia National Laboratories (SNL) developed the design analysis kit for optimization and terascale applications (DAKOTA) toolkit to compute uncertainties. The DAKOTA provides an interface for nuclear codes [12] and allows researchers to combine the objectives of the SA with the UP methods and determine the effects of the input parameters. The sampling models such as the Monte Carlo and Latin hypercube sampling (LHS) are implemented using this toolkit. The fuel codes, along with the DAKOTA, help perform the sensitivity and variance analyses.

3. IMPLEMENTATION OF UNCERTAINTY ANALYSIS

3.1 Fuel Performance Analysis

FRAPCON, a computer code used to determine the steady-state, thermal-mechanical behavior of oxide fuel rods for high burnup, is a fuel code used to study the thermo–mechanical behavior in permanent regimes, simulating a single fuel rod up to a burnup point of 62 GWd/MTU [13]. The fuel-rod analysis program transient (FRAPTRAN) is a system written using the FORTRAN language, to determine the transient performance of fuel rods in light water reactors (LWRs) during real or hypothetical accidents, when conditions are no longer those seen in the permanent regimes. FRAPCON and FRAPTRAN were developed at the Pacific Northwest National Laboratory (PNNL) during the 1970s [14]. The main objective of the fuel-performance codes is to evaluate the response of a fuel rod to either normal operating or transient conditions. The kinetic codes of the reactor are employed to calculate the assembly averaged neutron flux and power distributions, and subsequently, evaluate the potential transient conditions. The transient modeling establishes a dependency on the thermal properties of a system. Further, the uncertainties depend on the temperature and is influenced by the porosity and radiation.

3.2 Uncertainty Quantification of Physical Models

The NRC suggests a material library MATPRO for the thermal hydraulic (TH) system codes, which is the same as that employed for FRAPCON and FRAPTRAN. In the licensing process, use to nuclear units must utilize a system approved by NRC as FRAPCON containing eight physical models of uncertainty analysis can be used. The code permits direct additions to the input file using individual variables in the system. Thus, it is simple to use the FRAPCON with eight physical models for construction and application in the SA.

3.3 Uncertainty in Thermal Conductivity

Radiation damages the ceramic fuels, leading to trending changes in their physical properties. The thermal conductivity of UO_2 is reduced, thereby increasing the melting risk of the fuel rod. The process of heat transfer depends on the atomic diffusion of the fission products produced. The fission products that are diffused and stored are known to damage the crystals. At least five of the properties of uranium dioxide tracked in the thermal models are affected by this process, including thermal expansion, density, heat fusion, enthalpy, specific heat, and thermal conductivity. The thermal conductivity of the fresh fuel is a function of the temperature (T) in Kelvin, and can be calculated using Equation (1). The burning conditions affect the conductivity of UO_2, and composite fuels such as UO_2–BeO may exhibit high constituencies. The conductivity increases with the increase in the theoretical density and decreases with radiation (which causes damages). The temperature may change because of the heat conduction mechanisms; thus, it is among the influential factors. The conductivity decreases with the increase in the temperature up to 1726 °C, and subsequently, increases with temperature until a melting point of 2840 °C. The standard deviation of the calculated numbers, obtained from considering the causes discussed above, is generally considered 8.8%.

$$\lambda_0(T) = \frac{1-p}{1+cp}\left[\frac{1}{a+bT} + \frac{1}{T^{2.05}}\exp(d-\frac{e}{T})\right] \tag{1}$$

Here, λ_0 is the thermal conductivity of the un-irradiated fuel, and p is the porosity of the uranium dioxide. The fitted parameters, obtained from the experimental studies, are represented by *a, b, c, d,* and *e.*

Table 1: Uncertainty parameters of UO_2 thermal conductivity model

Parameter	μ (mean)	σ (sigma)
a (Gaussian)	5.574×10^{-2}	1.432×10^{-2}
b (Gaussian)	2.02×10^{-4}	1.215×10^{-5}
c (Uniform)	0.5	2
d (Gaussian)	23.847	0.9594
e (Gaussian)	2.034×10^{4}	2.714×10^{3}

3.4 Uncertainty in Thermal Expansion

Pellet fractures, formed predominantly by radial cracks, are a common result of thermal expansion. Such fissures occur because of the circumferential stress, which propagates toward the center of the pellet. The dimension of pellet often changes with the linear expansion of grain size used in the un-irradiated UO_2. In the thermal range of 1000 to 1500 °C, notable anomalous effects exist. The effect of the irradiation on the correlations is negligible. Therefore, the thermal expansion coefficient (CTE) is a function of the density and grain size. The fuel coefficient CTE helps in anticipating the mechanical contact between the pellet and the cladding for a standard deviation of 10.3%.

3.5 Fission-Gas-Release Model

The numerical result of the gas-diffusion equation is a practical solution used in the fuel codes. The noble gases xenon and krypton are products of nuclear fission. The heat transport during this process depends on the diffusion equation applied to the gas bubbles created in the fuel grains. The fission-gas-release equations describe a few sub-models, such as bubble growth and bubble coalescence, which have been the subjects of additional research.

At least five parameters of uncertainty are present in the physical model of this process, as listed in Table 4. The grain size of the uranium dioxide ranges between 20 and 100 µm with a variation of 60%, and the intra-granular diffusion coefficient factor is 100. The uncertainties associated with the intergranular diffusion coefficient can be determined using Equation (2). The grain-face boundary diffusion coefficient can be estimated using Equations (3), (4), and (5).

$$D_{ig} = D_1 + D_2 \tag{2}$$

$$D_1 = 7.6x10^{-10} \exp(-4.86x10^{-19}/(kT)) \tag{3}$$

$$D_2 = 1.41x10^{-25} \exp(-1.91x10^{-19}/(kT)) \tag{4}$$

$$D_{gb} = 8.86x10^{-6}\sqrt{F} \exp(-5.75x10^{-19}/(kT)) \tag{5}$$

where, D_1 (m^2s^{-1}), irradiation-enhanced diffusion is represented by D_2 (m^2s^{-1}), and F ($m^{-3}s^{-1}$) is the fission rate.

Table 2: Uncertainty parameters

Uncertainty parameter	Uncertainty range
Temperature (°C)	5%
Grain size, diameter (µm)	60%
Intra-granular diffusion coefficient, D_{ig}	Factor of 100
Intra-granular resolution parameter, b	Factor of 100
Grain boundary diffusion coefficient, D_{gb}	Factor of 100

The fission products, primarily xenon, create bubbles at the grain boundaries. These gas bubbles and inner-crystal lattice undergo a nucleation process, measured as a resolution parameter. The homogeneous model comprises a bubble-nucleation process based on a single gas atom at a time. The bubble size increases with the increase in the irradiation temperature. In Equation (10), the resolution parameter for the LWRs is expressed using a standard fission rate of F = 10^{19} (m^{-3} s^{-1}).

$$b = 10^{-23} F \tag{6}$$

3.6 Fuel-Swelling Models

The swelling of the fuel decreases as a function of the distance from the pellet centerline, depending on the temperature, burnup, and porosity. The effect of fission products, such as gaseous xenon and krypton, on the physical models is considerable. The fission gas release (FGR) leads to an increase in the pressure and decrease in the thermal conductivity of the gas filling the rod, which is typically helium. The variation in the gas-diffusion coefficient is 100%. The swelling of the fuel produces additional uncertainty depending on the fuel burn up, ranging from 0.08 to 0.16%.

3.7 Corrosion and Hydrogen Pickup Models

The fuel-rod corrosion rate is primarily a function of the time and temperature, and can be weakly represented as a function of the burn extension. At low temperatures, between 250 and 400 °C, oxidation occurs in two phases: a pre-transition oxidation process, which follows a cubic time dependence, and a post-transition stage, which follows a linear time dependency. The corrosion rate can be modeled to depend on the metallurgical manufacturing process of the zirconium alloys, ranging from 7.6 to 15 μm, or Zirlo, with an absolute value of 15 μm. Hydride models may instead have an absolute deviation in the range of 10–110 ppm.

3.8 Confidence Limits

The methodologies applied in the nuclear simulation are the Spearman's rank coefficient and sensitivity indices. DAKOTA helps in developing realistic, probabilistic models. The toolkit is used to calculate a statistical index such as the Pearson and Spearman's rank to measure the order correlations. When the distribution is free, the nonparametric approach is employed to evaluate the correlation between the two sets of parameters. A distribution-free approach results in a rank correlation between the related variables, wherein each set may be implemented for an order of magnitude. The sample used in this study comprised two hundred cases; thus, the confidence limit is improved. The BE models and SA execute a complex scheme using sets of random samples. Although the number of factors is considerable, only a small number of factors significantly affect the output of the model. Thus, using the applied methodologies, a small number of parameters are defined as key parameters, the effects of which on the model outputs are the highest for a wide range of engineering problems in the SA and optimization. The purpose of the SA is to investigate the connection between the inputs and responses obtained using the physical models. By performing the SA on the outputs of the nuclear-fuel code, it is possible to detect data with greater relevance and accuracy.

4. FRAMEWORK IMPLEMENTATIONS

4.1 Series IFA-650

In the Halden reactor program (HRP), sponsored by the OECD, 12 experiments were conducted reproducing the LBLOCA scenarios. The IFA-650 series performed LOCA experiments broadly investigating the behavior of high-burnup fuel under transient conditions. The test realized was an idealized fuel rod, using a few adaptations based on three fuel rods used in

LOCA series IFA-650-5, IFA-650-6 and IFA 650-7. The PWR fuel rod was pre-irradiated at 58 GWd/MTU and submitted at LOCA conditions, like the tests carried out in Halden program. The tested idealized is a fuel used in power water reactor. A fuel length of 0.47 mm with Zircaloy-4 cladding. The outer diameter was 9.50 mm, and the wall thickness was 0.75 mm, yielding a plenum volume in the range of 17 cm^3. The gas used to fill the system was a balanced mixture of 95% Ar and 5% He, pressurized at 4 MPa. The pellets were 4.48% enriched using uranium dioxide as fuel and Zircaloy-4 as cladding. The coating exhibited an embrittlement after irradiation because of a hydrogen uptake of roughly 380 ppm. The fuel rod underwent commercial cycles of 58 GWd/MTU. In the heating-up phase, the temperature increased abruptly from 200 °C to 1100 °C in approximately 310 s. A PCT of 850 °C was reached after 308 s from the initiation of the blowdown. The corroded outer surface produced a layer of zirconia with a thickness of 75 µm

4.2 Uncertainties applied

The fabrication tolerance represents the allowable variations in the dimensions such as form and size. The fabrication tolerances are the dimensional deviations created during the manufacturing process. In the modeling, these tolerances include the fluctuations in the fuel and rod size. The mechanical dimensions in question must be subject to random sampling using the propagation methods. The variations in the gap size could increase the risk of fragmentation and fuel relocation. Table 3 lists the manufacturing uncertainties.

Table 3: Normal distribution of manufacturing parameters

Uncertainty parameter	µ (mean)	σ (sigma)	Lower	Upper
Cladding outside diameter (mm), [dco]	9.5	0.95	9.405	9.595
Cladding inside diameter (mm),	8.36	0.0836	8.4436	2.2764
Cladding thickness (mm), [thkcld]	0.57	0.0057	0,5643	0.5757
Diametral gap thickness (mm), [thkgap]	0.150	0.00150	0.1485	0.1515
Fuel pellet diameters (mm)	8.21	0.0821	8.1219	8.2921
Fuel density (%) [td]	95.2	0.952	95.1048	95.2942
Fuel enrichment U-235 [enrch]	4.49	0.0449	4.4451	4.5349
Fuel rod pitch (mm), [pitch]	9.59	0.0959	9.4951	9.6859
Fill gas pressure (MPa), [fgpav]	4	0.04	3.96	4.04
Plenum length (cm), [cpl]	30.5	0.305	30.195	30.805
Temperature of sintered (C), [tsint]	1600	16	1584	1616
Increasing pellet density (Kg/m3) [rsntr]	100	1	99	101

Table 4 express the boundary conditions uncertainties used. Table 5 shown the uncertainties of physical models implemented by FRAPCON code. Such as Thermal expansion of UO_2, fission gas release model used for UO_2, creep model, hydride models, and others. Twenty inputs of uncertainties were applied for FRAPCON code as seven models included in the system code. Uncertainties models also used 1% of uncertainties such as thermal conductivity of UO_2 A confidence interval of 95% was used for the input variables; this was chosen because of the central limit theorem obtained by sampling the results from the executed modeling. In this simulation were executed 96 run codes using FRAPCON and FRAPTRAN.

Table 4: Boundary conditions

Uncertainty parameter	μ (mean)	σ (sigma)	Lower	Upper
Coolant inlet temperature (°C), [tw]	301.7	3.017	298.683	304.717
Mass flux of coolant (kg/s-m^2), [go]	26.52	0.2652	26.2548	26.7852
Coolant system pressure (MPa), [p2]	15.51	0.1551	15.35	15.46

Table 5: Uncertainties applied for physical models

Physical Models	Name	Bias
Bias fuel thermal conductivity model	sigftc	1%
Bias on fuel thermal expansion model	sigftex	1%
Bias on fission gas release model	sigfgr	1%
Bias on fuel swelling model	sigswell	1%
Bias on cladding creep model	sigcreep	1%
Bias on cladding axial growth	siggro	1%
Bias on cladding corrosion	sigcor	1%
Bias on cladding hydrogen pickup model	sigh2	1%

4.3 Steady State Sensitivity Analysis

Using 90 samples, and running FRAPCON detected that there are correlations identified as relevant, between the input and output variants. The identification process used the coefficients by Pearson and Spearman. In the case values, higher than 0.3 were walked with the five ranks of positions of Spearman's and confirmed. The graphs present the correlations identified during the of the burn cycle. Figure 1, showed Spearman rank correlation, that produced output changes with normal operations, such as gas pressure applied by helium and argon. Increasing internal pressure between fuel and cladding. Figure 2, described fuel surface temperature sensibility dependences from input uncertainties.

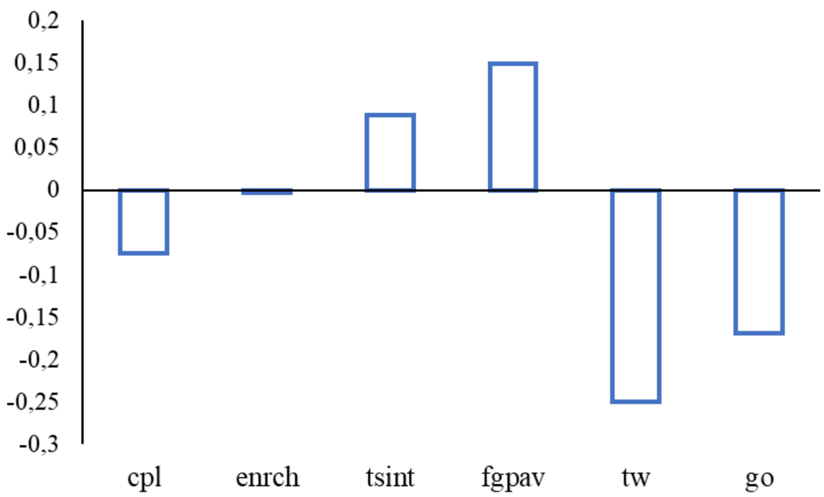

Figure 1: Spearman coefficients identified between interface pressure and inputs

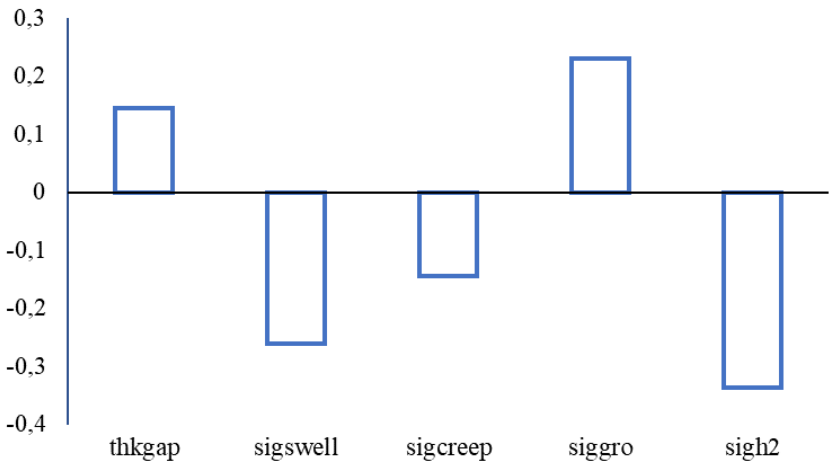

Figure 2: Spearman coefficients identified fuel surface temperature and inputs

4.4 Transient Analysis

The sensitivity analysis employed in the input variables using normal distribution we obtain outputs with tuned variations on 20% for most output variables. This result can be understood that the twenty output variables with 1% uncertainty should produce a higher change in the output, being able to create variations greater than 100%

Table 6: Uncertainties identified in the output parameters

Output parameters	Name	Uncertainties
Gap Interface Pressure	GIP	24.53%
Average fuel temperature	AFT	2.8%
Pellet surface temperature	PST	5.93%
Fuel centerline temperature	FCT	13.26%
Cladding inside temperature	CIT	4.26%
Cladding outside temperature	COT	4.0%
Cladding outside oxidation	COO	42,5%
Effective cladding stress	ECS	19.9%
Cladding hoop strain rate	CSR	77%
Fuel hoop strain	FHS	34.5%

We can notice that the uncertainties reach the pressure of the interface formed between the fuel pellet and cladding. Therefore, the temperature produced by fuel and cladding is a key factor that must be reduced to avoid accidents. During the transient, the input parameters that have the greatest influence on the output variables were the manufacturing uncertainties used. The thickness of the gap has a similar power compared with fuel external diameter, and the thickness variation thereof as shown in the fig. 3 and fig. 4. Variations in the hydraulic diameter (pitch) have an average sensitivity the fuel and cladding temperatures. The external temperature of the fuel was which indicates greater sensitivity compared to the others listed in the table 6.

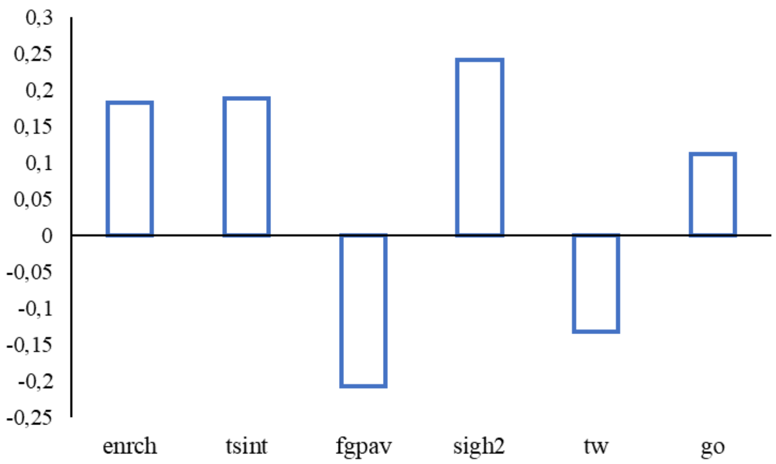

Figure 3: Spearman coefficients identified cladding outside temperature and inputs

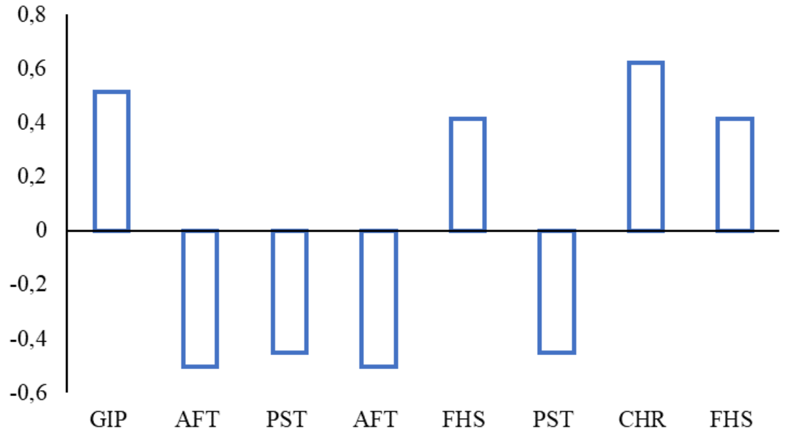

Figure 4: Spearman coefficients produced cladding outside diameter

5. CONCLUSION

The proposed model was used to integrate the fuel performance system with the DAKOTA toolkit. A case study was conducted on a LOCA by directly integrating the SA using the Spearman index. The statistical distributions used to implement the model were built using DAKOTA, based on the mean values and deviations of the variables. In the simulations, we note that small variations introduced in the input parameters were propagated to the output. As the number of simulations increased, there was a strong tendency to increase the uncertainty in the output parameters. In the case where the number of simulations reaches 196 run codes, we must obtain greater variations, but we must better identify the sensitivity of the set of variables used. The licensing code FRAPCON, combined with FRAPTRAN, was used to construct 96 cases for testing and analysis. In a similar research, FRAPCON was used to develop the SA with internal models for uncertainty propagations. The sampling was done based on the effects due to the manufacturing tolerances combined with the boundary conditions. The large sources of uncertainty, requiring the SA, include the uncertainties described in the physical models. The proposed modeling and methodology were used to predict the results of the fuel rod experiment idealized, the results of which are presented in this study.

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