Global Sensitivity Analyses on Coupled VERA-CS/BISON and VERA-CS/FRAPCON Simulations

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INTRODUCTION

The prediction of the fuel behavior of light water reactors under both normal and abnormal operating conditions is very challenging because it involves predicting the interacting and competing multi-physics phenomena pertinent to nuclear, thermal, mechanical, chemical and fluid flow processes. The models developed for these complex physical processes are often non-linear with multiple scales in space and time, and with various mathematical models and parameters. Hence uncertainties have to be considered in multi-physics simulations of fuel performance. Consequently, for applications of multi-physics simulations, proper uncertainty quantification (UQ) and sensitivity analysis (SA) of the mathematical models are important to comprehensively understand the results. Sensitivity analysis seeks to determine the contribution of the uncertainty in a single model input to the uncertainty in model results. It provides a clearer picture of how system inputs correlate to system outputs.

The objective of this work is to develop a sensitivity analysis methodology and perform comparative studies for coupled simulations of VERA-CS/FRAPCON and VERA-CS/BISON under steady state conditions. VERA-CS is a coupled neutronics/thermal hydraulics core simulator code developed by the Consortium for Advanced Simulation of Light Water Reactors (CASL) [1]. FRAPCON is NRC's fuel performance code developed by the Pacific Northwest National Laboratory (PNNL) [2] and BISON is an advanced fuels performance code being developed at Idaho National Laboratory [3]. There exist numerous sensitivity analysis methods that should be carefully chosen based on the complexity and specific model to be evaluated. Global sensitivity analysis methods explore the whole input parameter space by sampling chosen input parameters simultaneously rather than performing perturbations of input parameters one-at-a-time. Global sensitivity analysis has the advantage of being able to identify nonlinear uncertainty structures over the global admissible input parameter space. The non-influential parameters in nonlinearly parameterized models can be fixed for subsequent model calibration or uncertainty propagation. In this work, a Monte Carlo, or sampling based, approach is used to evaluate those parameters that most profoundly affect the figures of merit. In Monte Carlo based methods, a large number of model simulations are performed to produce a significant number of samples that can be used for both uncertainty quantification and sensitivity analysis.

PROBLEM DESCRIPTION

The test case under study is a depletion case for a single fuel assembly lasting four and half years or three cycles for a typical pressurized water reactor (PWR). A 17×17 PWR fuel assembly containing 264 fuel rods, 24 guide tubes and 1 instrumentation tube is modeled with VERA-CS. VERA-CS takes into account core and fuel assembly properties such as the upper and lower core plates, lower and upper assembly nozzles, and guide/instrument tubes. Eight spacer grids are included in the assembly to provide structural support as well as improve coolant mixing. The fuel performance computer codes are normally developed to analyze the behavior of a single fuel rod. Both FRAPCON and BISON are best estimate fuel performance codes that can calculate the response of light water reactor fuel rods under both the steady-state and transient conditions. Boundary conditions such as the fuel irradiation power history and axial power shapes, calculated by VERA-CS, are supplied as input to the codes. The FRAPCON and BISON calculations are performed only for the hot rod which is identified as the highest power rod in the assembly at the end of the VERA-CS depletion calculations. Performing fuels performance calculations only on the hot rod resulted from the runtime limitation of BISON.

Great care must be taken to assure consistent uncertainty propagation. The precise methodology is greatly dependent upon runtime and available resources. If the workload of codes is above or near the limit of available computational resources, then large samples are not attainable. In such cases, probability density functions (PDF) of outputs of interest are estimated from a limited sample size. Codes not hindered by hardware constraints may then use large sample sizes which are generated from the aforementioned PDFs. Fortunately, the high performance computer (HPC) resources at INL far exceed the required power for a single assembly VERA-CS case. Thus a large number of runs in VERA-CS for one assembly followed by FRAPCON and BISON runs for the hot rod are feasible. This method negates the need for intermediate PDF generation and resampling. In addition, the direct connection structure will be of great use in future work involving feedback between the codes. A schematic of the data flow is shown in Figure 1 with rectangular boxes representing files and elliptical shapes indicating programs.

The interface between VERA-CS and FRAPCON/BISON is done within the multi-physics best estimate plus uncertainty (MP-BEPU) analysis framework LOTUS [4]. The process begins by creating a list of perturbed inputs. The first set of LOTUS scripts combines perturbed inputs specific to VERA-CS with a VERA-CS input template to create an input file for each set of perturbed inputs. After a VERA-CS run for each input file, the second set of LOTUS scripts creates FRAPCON and BISON input files from VERA-CS output files, perturbed inputs specific to FRAPCON and BISON, and a FRAPCON and BISON template file.

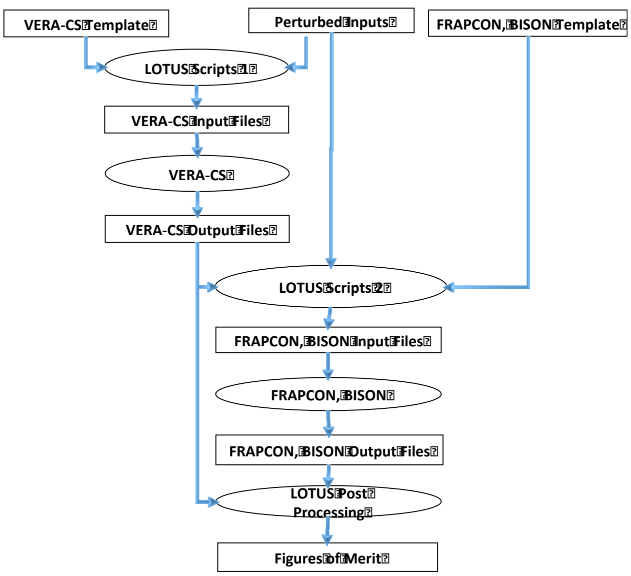

Fig. 1. Data Flow Structure for VERA-CS/FRAPCON and VERA-CS/BISON.

The data transferred from VERA-CS to FRAPCON include power shapes, inlet temperature, outlet pressure, and mass flow rates, and the data transferred from VERA-CS to BISON include power shapes and clad outer surface temperatures. It is worth noting that VERA-CS output files contain all VERA-CS input data as well. Hence any shared data is supplied to VERA-CS first, and then later retrieved from the VERA-CS output files before being supplied to FRAPCON and BISON.

After all FRAPCON and BISON cases are executed, LOTUS post processing scripts retrieve all figures of merit (FOM) data from both VERA-CS/FRAPCON, and VERA-CS/BISON output files. Lastly all UQ and SA metrics are calculated for the hot fuel rod.

The data flow structure between VERA-CS and FRAPCON/BSION is a loose coupling, meaning that there is no feedback between the two codes. For the quasi-steady state analyses carried out in this work, the loose coupling approach is adequate. However, for transient calculations, such as under LOCA conditions, strongly coupled calculations will be required. This is left for future work.

For the coupled VERA-CS/FRAPCON simulations, 23 parameters were selected as shown in Table 1 with "X" indicating the perturbed input parameters used by VERA-CS and/or FRAPCON. The star (*) in Table 1 denotes an input that very strongly affects a FRAPCON input, though it is not a direct input. The core power for instance, directly impacts the linear heat generation rate input of FRAPCON. Likewise, the mass inlet flux of FRAPCON is a result of the rated flow inputted to VERA-CS. The table positions with '-' entries, indicate that a nominal value does not exist in the FRAPCON code. Values such as fuel thermal conductivity vary greatly and are routinely updated. FRAPCON allows for manipulations of these values by biasing all calculation of the variable by a specified amount.

TABLE I. Uncertain Input Parameters for VERA-CS/FRAPCON Coupled Simulations (FRAP means FRAPCON)

Input Name	Nominal Value	Range (+/-)	VERA -CS	FRAP
Inlet Temperature	554.9 °F	3.0 °F	X	X
Outlet Pressure	15.513 MPa	2%	X	X
Fuel Radius	0.4096 cm	0.001 cm	X	X
Clad Inner Radius	0.418 cm	0.002 cm	X	X
Clad Outer Radius	0.475 cm	0.002 cm	X	X
Fuel Density (% Theoretical)	94.5%	1.6%	X	X
Fuel Enrichment (% Weight)	4.8%	0.003%	X	X
Direct Mod. Heating Fraction	0.02	10%	X	X
Assembly Power Cycle 1 Cycle 2 Cycle 3	 17.674 MW 13.256 MW 8.837 MW	2%	X	*
Rated Flow	3.410 Mlbs/hr	2.0%	X	*
Mid Spacer Grid Form Loss	0.9070	20%	X	
End Spacer Grid Form Loss	0.9065	20%	X	
Void Drift Coefficient	1.4	10%	X	
Turbulent Mixing Coefficient	0.005	10%	X	
Plenum Fill Gas Pressure	1.207 MPa	2.0%		X
Fuel Thermal Conductivity	-	10%		X
Fuel Thermal Expansion	-	15%		X
Fission Gas Release	-	+200%/ -67%		X
Fuel Swelling	-	20%		X
Cladding Creep	-	30%		X
Cladding Axial Growth	-	50%		X
Cladding Corrosion	-	40%		X
Cladding Hydrogen	-	80 ppm		X

For the coupled VERA-CS/BISON simulations, 31 parameters were selected. Due to the page limitation, the table of uncertain parameters is omitted.

REGRESSION, VARIANCE, AND DENSITY BASED GLOBAL SENSITIVITY ANALYSIS METHODS

Regression Based Sensitivity Measures

Pearson correlation coefficients are a regression based measure. A useful visualization of regression methods is the passing of a straight line through a scatterplot of the data. If all the data lies perfectly on the fitted line, the Pearson measure is unity. If all straight lines have no bearing on the data (excluding lines with zero slope), then the measure is zero. Pearson correlation coefficients may be thought of as a normalized covariance of an output and input, and are found by Equation 1,

$$R_i^2 = \frac{cov(X_i,Y)^2}{var(X_i)var(Y)} \tag{1}$$

The Pearson measures do allow for an assessment of the linearity of the system. For a purely linear system, the sum of all Pearson values ($\sum_{i=1}^{N} R_i^2$) is unity, with increases in nonlinearity resulting in a sum closer to zero.

A natural extension of the Pearson measure is the Spearman correlation coefficients. Spearman differs in that it evaluates the rankings of inputs and outputs as opposed to the actual values. Spearman is advantageous over Pearson in that it is superior in detecting nonlinearities, as long as the relations are monotonic.

Variance Based Sensitivity Measures

Sobol variance decomposition method is a variance based measure, which entails comparing the contribution of one input to the variance of an output. Sobol indices differ from Pearson correlation coefficients in that Pearson measures are based upon linear regression, while Sobol indices capture more complex interactions. Here only the first order terms are presented. Sobol indices are expressed mathematically in Equation 2,

$$S_i = \frac{var\left(E_{X_i}\left(Y_{Y|X_i}\right)\right)}{var(Y)} \tag{2}$$

where S_i is the Sobol indices, and $E_{X_i}()$ is the expected value operator, expanded below in Equation 3,

$$E_{X_i}\left(var\left(Y_{Y|X_i}\right)\right) = \int f_{X_i}(x_i)\, var\left(Y_{Y|X_i}\right) dx_i \tag{3}$$

Sobol indices are computationally expensive. The sum of Sobol indices lies between zero (non-additive) and unity (additive). It is important to note that a sum of unity does not necessarily indicate linearity. If the definitions in Equations 2 and 3 are strictly adhered to, a double loop Monte Carlo method is required, as opposed to the more random sampling typically used for Pearson measures. Plischke method allows for the partitioning of a typical random distribution into approximately equally spaced partitions based upon the rankings of a given input [5]. Estimators for the Sobol indices can be recast as Equation 4,

$$\widehat{S_i} = \frac{\frac{1}{N}\sum_{j=1}^{M} N_j var\left(Y_{Y|x_i \in X_j}\right)}{var(Y)} \tag{4}$$

where X_j represents a partition of the sample with a population of N_j, M is the number of partitions, and N the total sample size. In order to reduce bias, the boot strapping method is used with 10 resamples with replacement. Sobol indices were calculated using the SA Library in Python [6].

Density Based Sensitivity Measures

Density based moments are independent of the moments of the data (i.e. mean and variance). The delta moment independent measures are a recent metric established by Borogonovo [7]. The delta measure is based upon the expected L^1 norm differences between conditional and unconditional probability density functions for a given input. This is expressed mathematically in Equations 5 and 6.

$$s(X_i) = \int \left| f_Y(y) - f_{Y|X_i}(y) \right| dy \tag{5}$$

$$\delta_i = \frac{1}{2} E_{X_i}\left(s(X_i)\right) = \frac{1}{2}\int f_{X_i}(x_i) s(x_i)\, dx_i \tag{6}$$

where $s(X_i)$ is the L^1 norm between the unconditional density $f_Y(y)$ and the conditional density $f_{Y|X_i}(y)$, $E_{X_i}()$ is the expected value operator, and δ_i is the delta moment independent measure. The delta measure is advantageous in that it is density based. As a result, complex relations that effect distribution but not necessarily variance, are captured. The summation of all delta indices is between zero and unity. Sums close to unity indicate that the contributions from a group of inputs on an output are separable from each other, while lower sums indicate the shifts in distribution are inseparable.

As with the Sobol method, Delta measures ideally use a double loop Monte Carlo method. The partitioning strategy [5] presented in aforementioned Sobol Indices subsection is used to recast Equations 5 and 6 as Equations 7 and 8.

$$s\left(x_i \in X_j\right) = \int \left| f_Y(y) - f_{Y|x_i \in X_j}(y) \right| dy \tag{7}$$

$$\widehat{\delta_i} = \frac{1}{2N}\sum_{j=1}^{m} N_j s\left(x_i \in X_j\right) \tag{8}$$

The integral used in Equation 7 is estimated via kernel density estimators. While a variety of kernels are available, this work uses the more common Gaussian kernels, with future work planned to implement the more recent diffusion kernels. Bootstrapping methods are used for delta indices as well, with 10 resamples with replacement. Delta measures were calculated using the SA library in Python [6].

RESULTS

The SA simulations were performed on the Fusion supercomputer at the INL. The figure of merit (FOM) for this study is gap conductance at peak power (GCPP). The LOTUS toolkit was used to create 2500 VERA-CS/FRAPCON and VERA-CS/BISON input files with perturbed parameters outlined by the tables of uncertain parameters shown in Table 1. All the 2500 VERA-CS/FRAPCON and VERA-CS/BISON cases run successfully and are considered here. The LOTUS post-processor was then used to extract the FOMs, perturbed values, and any other quantities of interest to perform SA.

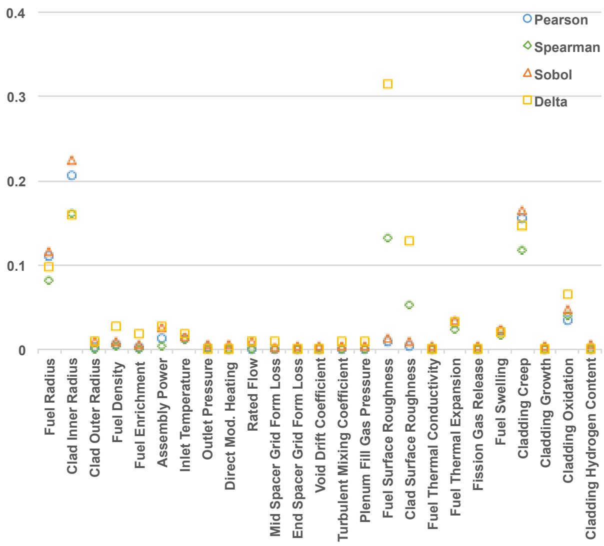

Fig. 2. SA Measures for GCPP from VERA-CS/FRAPCON Calculations at 348 Days in Fuel Cycle.

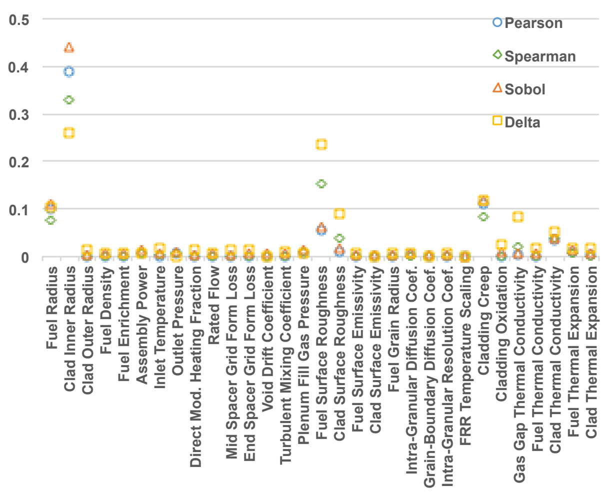

Fig. 3. SA Measures for GCPP from VERA-CS/BISON Calculations at 348 Days in Fuel Cycle.

At low and high burnup states, SA measures show strong agreement between VERA-CS/FRAPCON and VERA-CS/BISON simulations. For intermediate burnup states such as at 348 days, the SA measures are shown in Figures 2 and 3. This is the first recorded state that contains significant interfacial pressure for some instances of the Monte Carlo sampling. The state contains a relatively large amount of nonlinearities as both codes switch from a dependence on gap dimensions to fuel and cladding surface roughness in addition to cladding creep and oxidation, fuel swelling and thermal expansion. While all aforementioned inputs play significant roles in each code, the ranking and magnitudes of the measures differ between codes. Note also that some inputs of minor impact in BISON for this state could not be perturbed in FRAPCON, thereby adding to differences in results.

SUMMARY

The behavior of GCPP in FRAPCON and BISON for a single PWR fuel assembly depletion case was elucidated through the LOTUS toolkit. Sensitivity analysis results for GCPP are largely consistent in terms of sharing the same impactful inputs, but often differ in their magnitude and ranking, particularly at the initial onset of interfacial pressure.

ACKNOWLEDGMENTS

This work is supported by the U.S. Department of Energy, under DOE Idaho Operations Office Contract DE-AC07-05ID14517. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

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