SENSITIVITY ANALYSIS BY THE USE OF A SURROGATE MODEL IN LB-LOCA: LOFT L2-5 WITH CATHARE-2 V2.5 CODE

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ABSTRACT

The revision of the 10 CFR50.46 in 1988 has made possible the use of best-estimate (BE) codes in safety demonstration and licensing, provided that uncertainties are added to the relevant output parameters before comparing them with the acceptance criteria. In the safety analysis of the large break loss of coolant accident, for a BE analysis, it was agreed that the 95th percentile estimated with a high degree of confidence should be lower than the acceptance criteria. It appeared necessary to IRSN, technical support of the French Safety Authority, to get more insight into these strategies.

The application of the BE plus uncertainty analysis can be made in three steps in a statistical evaluation:
- The definition and the evaluation of uncertainties of the input parameters;
- The modelling and understanding of the output parameters;
- The evaluation of the 95th percentile with a high degree of confidence.

As a general rule the global sensitivity analysis (GSA) is done with linear correlation coefficients. This paper presents a new approach to perform a more accurate GSA to determine and to classify the main input parameters. Such information is difficult to obtain directly by Monte-Carlo methodologies using the thermal-hydraulic code, because it is rather time-consuming. Therefore, it is natural to replace it with a simpler model called a surrogate model too. We suggest Kriging methodology for its construction and the SOBOL methodology for the GSA.

The paper presents the application of the previously described methodology on the LOFT (Loss-of-Fluid Test) loss of coolant experiment L2-5 which simulated a double-ended offset shear of a cold leg in the primary coolant system. LOFT L2-5 has been the subject of the BEMUSE international problem. The output is the first maximum Peak Cladding Temperature of the fuel. The best estimate code used is CATHARE2 V2.5.

KEYWORDS
Response surface methodology, Kriging, Simulated annealing, Sensitivity analysis, Sobol

1 INTRODUCTION

The methods using best estimate codes, associated with an evaluation of uncertainties related to the relevant output parameters, will be used much more than ever in safety demonstration for nuclear power plants (NPP). In order to develop a method of uncertainty propagation and to get more insight to these methodologies, IRSN chose, in a first step, to apply it to the calculation of the LOFT L2.5 experiment (simulation of a double-ended offset shear of a cold leg in the primary coolant system). In our study, we will be mainly focusing on the relevant output parameter which corresponds to the first maximum peak cladding temperature (PCT) of the fuel during the transient.

In order to evaluate the PCT, we use the best-estimate code CATHARE2 V2.5, a thermal hydraulics code developed by CEA, IRSN, EDF and FAMATOME for PWR safety analysis. The PCT depends on 42 input parameters whose uncertainties have been estimated by the IRSN and CEA experts in thermal hydraulics. In this paper, we try to quantify the influence of each uncertain input parameter on the response variability of the numerical model with a global sensitivity analysis (SA). Global SA focuses on the output uncertainty over the entire range of variations of the input parameters. We propose the famous and powerful Sobol' approach, which is a variance-based method, to evaluate how the variance of an input contributes into the variance of output.

Toward the objective of assessing uncertainty, it is useful to further analyse the PCT. For instance, one would like to trace the sensitivity of the PCT to each input parameter, or to determine the situations that result in high temperatures. Such information is difficult to obtain using the CATHARE code, because it is quite time-consuming and too time expensive to apply directly the global SA methods. Therefore, it is natural to replace the complex computer code CATHARE by an approximate mathematical model, called response surface or surrogate model. The response surface method is used to build a function which simulates the behaviour of a physical or chemical phenomenon, starting from a certain number of experiments and in our case for computer case.

This function must be as representative as possible of the computer code, with good prediction capabilities and must require a negligible calculation time. Several response surfaces are classically used: polynomials, splines, neural networks, kriging,... We propose in this paper the kriging approach for the construction of response surface.

This paper is organized as follows. In section 2, we present the approaches for the construction of response surfaces and for the sensitivity analysis, and apply them to the modelling of the PCT. Results are presented in section 3. Finally, concluding remarks in section 4.

2 MODEL FOR THE CONSTRUCTION OF RESPONSE SURFACES

For this section, we will assume that we have obtained the outputs of n runs by the CATHARE code. Each run corresponds to a vector of some input parameters values $x_1,\ldots,x_k$. We call that

vector a point and we denote it by a bold letter $\boldsymbol{x} = (x_1,\ldots,x_k)$. The n points corresponding to the runs are called an experimental design and will be denoted $(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$. The CATHARE code can be viewed as a function y_{sim}. Denote $y^{(1)},\ldots,y^{(n)}$ the outputs corresponding to the runs: $y^{(i)} = y_{sim}(\boldsymbol{x}^{(i)})$, $i=1,2,\ldots,n$. Since we cannot use directly the costly function y_{sim}, we want to use the knowledge that we get at $(\boldsymbol{x}^{(1)},\ldots,\boldsymbol{x}^{(n)})$ to model it the most accurately as possible. This problem can be addressed in using an interpolation technique: the kriging method.

2.1 Experimental design

The quality of the response surfaces depends on the choice of the experimental design. This explains why there is a huge literature on the topic, mostly devoted to physical experiments. The specificities of computer experiments have led to new designs, named *Latin hypercube designs* [**3**], that ensure little redundancy of design points when some of the input parameters have a small effect on the output. Some of them have, in addition, good optimality and orthogonallity properties. The optimality property guarantees the estimation quality, and the orthogonallity property ensures that the effects of input parameters are distinguishable. For instance, Butler [**1**] shows how to construct Latin hypercube designs with good properties when the model is a second order polynomial linear regression (this assumption is currently done by statisticians). However, we do not know a similar construction for kriging. We have decided to use the Latin hypercube design suggested by Butler [**1**]. Even if we have no idea about optimality and orthogonallity in the kriging case, the results obtained with this design are encouraging.

2.2 Interpolation model: kriging

Doing computer simulations is very different than doing a physical experiment. Firstly, the repetition of a computer experiment should always give, theoretically, the same result. In addition, the simulator solves some differential equations, and may deduce the value at a point in the factors domain from neighbouring values. Therefore, high spatial correlation is expected between two near points. These two characteristics have led to the introduction in the 90's of another model with interpolation and spatial correlation properties [**4**], [**5**]. Actually, this model was initially introduced in dimension 3 in geostatistics by Krige, and is known since as kriging model. It can be written as:

$$y_{\text{sim}}(\boldsymbol{x}^{(i)}) = \sum_h f_h(\boldsymbol{x}^{(i)})\beta_h + Z(\boldsymbol{x}^{(i)}), \quad i = 1,2,\ldots,n \tag{1}$$

The mathematical expression is not so far from linear regression, but assumptions on errors are very different: $Z(\boldsymbol{x})$ is a centred (Gaussian) stationary stochastic process with "distance"-decreasing correlation function. It means that the correlation between $Z(\boldsymbol{x})$ and $Z(\boldsymbol{y})$ is a decreasing function of the "distance" between x and y. In this paper, we will use the power exponential covariance structure, given by:

$$\mathrm{cov}(Z(\boldsymbol{x}), Z(\boldsymbol{y})) = \sigma^2 R(\boldsymbol{x}-\boldsymbol{y}) = \sigma^2 \exp\left(-\sum_{h=1}^{k} \theta_h \mid x_h - y_h \mid^{p_h} \right) \quad (2)$$

where:

$\theta_1,\ldots,\theta_k$ are positive real numbers.

$p_1,\ldots,p_k$ are positive real numbers lower or equal to 2 (this condition ensures that all covariance matrices are definite positive).

In this modelling, the simulator can be viewed as a particular (deterministic) path of the process. Its shape and regularity depend on the parameters of the covariance structure. More precisely the θ_h's are spatial frequency parameters: a small value in a direction is synonym with low frequency. The p_h's are regularity parameters. The nearer p_h is to 2, the smoother the response surface is. To illustrate this fact, we have drawn in Figure 1 below the paths corresponding to three different values of p in dimension 1 ($k = 1$). In practise, all these parameters are unknown; they are estimated by maximizing the model likelihood with simulated annealing method.

Finally, the functions f_h's have to be chosen. But with this model, it seems that the assumptions on the correlation structure are "so powerful" that we can choose a constant [**2**]. Thus, we have decided to use the model (3):

$$y_{\mathrm{sim}}(\boldsymbol{x}^{(i)}) = \mu + Z(\boldsymbol{x}^{(i)}) \quad (3)$$

2.3 Optimization: simulated annealing

Simulated annealing [**6**] found its origins in thermodynamics. This method results from an analogy between the physical phenomena of slow cooling of a body in fusion, which leads it to a solid state, of low energy. The temperature should be lowered slowly, by marking sufficiently long stages so that the body reaches "thermodynamic balance" with each stage of temperature. For materials, this low energy appears by obtaining a regular structure, as in the crystals and steel.

The analogy exploited by simulated annealing is considering a function f to be minimized like function of energy, and a solution $\boldsymbol{x}$ can be regarded as a given state of the matter whose energy is $f(\boldsymbol{x})$. Simulated annealing generally exploits the criterion defined by the algorithm of Metropolis [**7**] for the acceptance of a solution obtained by disturbance of the current solution.

For a given "temperature" T, starting from a current solution $\boldsymbol{x}$, one considers an elementary transformation which would change $\boldsymbol{x}$ into $\boldsymbol{x}'$. If this disturbance induces a reduction in the value of the objective function f, $\Delta f = f(\boldsymbol{x}') - f(\boldsymbol{x}) < 0$, it is accepted. In the contrary case, if $\Delta f = f(\boldsymbol{x}') - f(\boldsymbol{x}) > 0$, the disturbance is accepted all the same with a probability $p = \exp(-\Delta f / T)$.

The controlling parameter T is the "temperature" of the system, which influences the probability of accepting a worse solution. With a high temperature, the probability of acceptance of an unspecified movement tends towards 1 (almost all the changes are accepted). The algorithm is

equivalent then to a random walk in the space of the configurations. This temperature is decreased slowly to simulate the process of cooling of materials, and its reduction is sufficiently slow so that thermodynamic balance is maintained.

The effectiveness of simulated annealing strongly depends on the choice of its controlling parameters, whose adjustment remains very empirical. The principal controlling parameters are the law of disturbance of the solution, the initial temperature, the temperature reduction function, the criterion of change of stage of temperature, and criteria of stop.

With each iteration i of the algorithm, an elementary modification or disturbance of the solution is carried out. In practice, the new candidate is simulated by the means of a random number U drawn according to a standard normal law:

$$x_{i+1} = x_i + \lambda \times U \tag{4}$$

The choice of the constant λ is of primary importance. Indeed, a strong value (> 1) of this coefficient will make it possible to quickly move over the entire range of model inputs. On the other hand, a low coefficient (< 0.1) will bring a profit of precision on the optimal solution, subject to a sufficient iteration count.

The role of the temperature T during the process of simulated annealing is very important. A large decrease of temperature is likely to trap the algorithm in a local minimum, whereas a small decrease at the beginning of the process will lead to a very slow convergence of the algorithm. A compromise is being adapted for the decrease of the temperature to the evolution of the process which consists of using a variation logarithmic curve. The logarithmic law of decrease of the temperature, which ensures the theoretical convergence of simulated annealing, is as follows:

$$T_k = \frac{\alpha}{Log(1+i)} \tag{5}$$

where i is the number of temperature stages carried out, and α a positive constant.

In practice, we often adopt a geometrical decrease $T_{i+1} = \alpha T_i$, with $(0.8 < \alpha < 1)$, because the preceding law induces a prohibitive computing time. For the change of stage of temperature, one can simply specify a number of transformations, accepted or not, with the end of which the temperature is lowered.

2.4 The response surface

To define the response surface constructed by kriging, we have to add the interpolation constraint: $y(\mathbf{x}^{(i)}) = y^{(i)}$, $1 \le i \le n$. Then, as for regression, the response surface is the best linear unbiased predictor. The derivation of its expression is not straightforward, and can be found in [**5**]. The predictor $y_{pred}(\mathbf{x})$ can be seen as a particular path of the (estimated) kriging process, interpolating the experimental points: $y_{pred}(\mathbf{x}^{(i)}) = y^{(i)}$, $1 \le i \le n$. More details and examples can be found in [**2**].

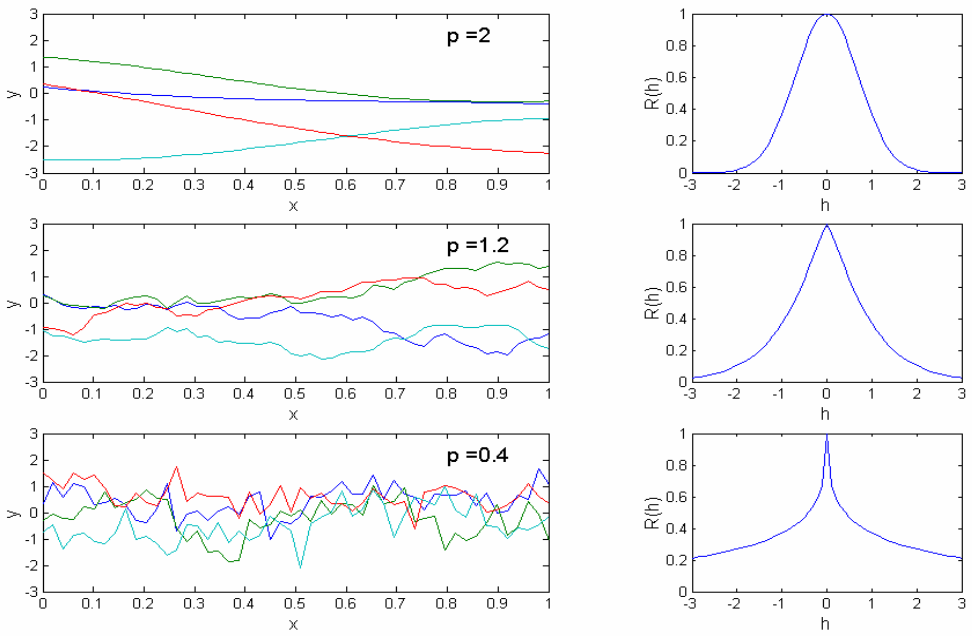

Figure 1. Examples of paths generated with the stochastic process *Z(x)* utilizing three different values of the regularity parameter: *p*=2, *p*=1.2 and *p*=0.4

2.5 Sensitivity analysis: Sobol' approach

Sensitivity analysis (SA) of a model output aims to quantify the relative importance of each input model parameter in determining the value of an assigned output variable. Global SA focuses on the output uncertainty over the entire range of values of the input parameters. The main idea of variance-based methods is to evaluate how the variance of an input or a group of inputs contributes into the variance of output.

Among the variance-based global methods, the approach of SOBOL makes it possible to estimate the fraction of variance of the response code explained by one of the input parameters. The main idea behind this approach is the decomposition of the function of the input parameters into summands of increasing dimensionality. It does not make any assumption on the model, but requires the independence of the input parameters.

In order to study the impact of the independent input parameters $\boldsymbol{x} = (x_1,\ldots,x_k)$ on the variance of the output $y = f(x_1,\ldots,x_k)$, we can compare the variance of y namely $V(y)$ with the conditional variance of y with x_i fixed to its true value x_i^*, $V(y \mid x_i=x_i^*)$. Unfortunately, in general the true values of the input parameters are not known. Therefore, a solution is to study the conditional expectation $E[V(y \mid x_i)]$, whereby it is built into all possible values of x_i.

The sensitivity indices of Sobol are given by (see [**8**] for more details):

$$S_i = \frac{V[E(y \mid x_i)]}{V(y)} \qquad S_{ij} = \frac{V[E(y \mid x_i, x_j)]}{V(y)} - S_i - S_j \qquad (6)$$

The first order sensitivity indices S_i measure the main effect of each unknown parameter x_j on the output y, or the fraction of variance of y due to the variance of x_i alone.

The second order indice S_{ij} expresses sensitivity of the model to the interaction between the variables x_i and x_j, (without the individual effects of x_i and x_j), and so on for the third, and higher order effects.

Finally, we define the total sensitivity indice of variable x_i which is defined as the sum of its all sensitivity indices, its main effect as well as all the higher order effects in which this value appears:

$$S_{T_i} = S_i + \sum_{1 \le j \le k,\, j \ne i} S_{ij} + \ldots + S_{1,2,\ldots,k} \qquad (7)$$

SOBOL proposes to estimate the sensitivity indices by a method of Monte Carlo which consists in simulating input variables and to estimate an integral by a sum of Riemann on these simulations ([**8**]).

3 RESULTS

In this section, we present results of our approach for the construction of response surface to the modelling of the first maximum PCT (see Figure 2), and results of the sensitivity analysis.

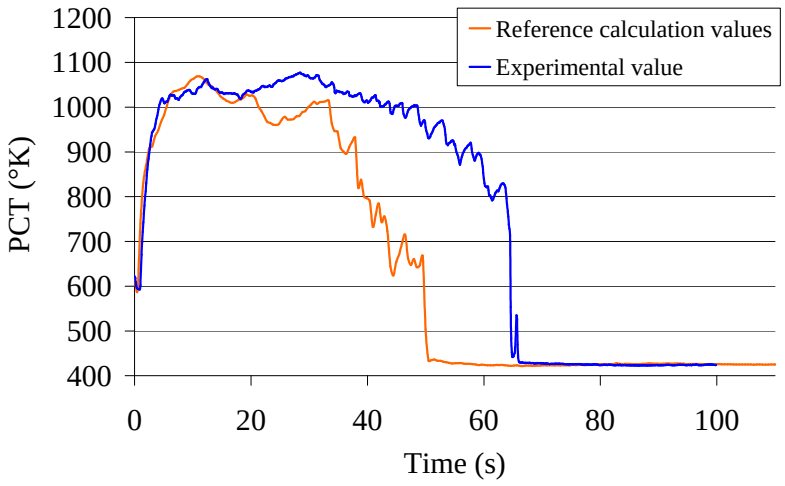

Figure 2. ***Temporal evolution of the PCT***

Actually, this study (kriging and sensitivity analysis) was carried out 2 times: the first time, we applied the kriging method with 42 input parameters and we used a coarse Sobol' analysis (with N = 50,000 Monte-Carlo iterations) in a prior-design stage to screen out variables that are probabilistically insignificant, and the second time to obtain precise results of sensitivity (with N = 400,000). Thus, we reduced dimension (and time of calculation) selecting 11 input parameters which will be considered in this section (Table I): Initial power, Gap size, Residual power, UO_2 conductivity, UO_2 specific heat, Film boiling, Vapour-wall friction, Interfacial friction, Vapour-wall heat transfer, Vapour-wall heat flux, and Bubbles raise velocity.

Table I. Uncertainty of input parameters

Input Parameter	**Initial power**	**Gap size**	**Residual power**	**UO_2 conductivity**	**UO_2 specific heat**	**Film boiling**
Uncertainty	[0.97;1.03]	[0.8;1.2]	[0.9;1.1]	[0.8;1.2]	[0.8;1.2]	[-42;60]

Input Parameter	**Vapour-wall friction**	**Interfacial friction**	**Vapour-wall heat transfer**	**Vapour-wall heat flux**	**Bubbles raise velocity**
Uncertainty	[0.8;1.9]	[0.6;1.8]	[0.5;2]	[0.15;6.5]	[0.4;5]

Most of the uncertainty ranges used are estimated by expert judgement. Afterwards, some of the uncertainties are also fitted by experimental comparison. The whole fitting of the uncertainty ranges against the Cathare code validation matrix experiments requires a lot of resources

3.1 Response surface

To build the response surface considering 11 input uncertain parameters, we used a 121 point Latin hypercube design. Its construction was carried out according to the method clarified in [**1**]. The estimated results obtained with simulating annealing approach are presented in Table II. The first line gives the parameter number h, and the two lines below the corresponding estimated values of the frequency parameters θ_h and regularity parameters p_h.

These unknown parameters are estimated by maximizing the model likelihood with simulated annealing method with controlling parameters as follows:

- law of disturbance of the solution: $x_{i+1} = x_i + 0.01 \times U$, with U a random number in [0;1];
- temperature reduction function: $T_{i+1} = 0.99 \times T_i$, with initial temperature T_0 = 2000;
- criteria of stop: 25,000 iterations.

Table II. Results obtained by kriging

Input Parameter	Initial power	Gap size	Residual power	UO_2 conductivity	UO_2 specific heat	Film boiling
Estimated θ_h	0.48	0.11	0.03	0.51	0.58	0.25
Estimated p_h	1.87	2	2	2	2	2

Input Parameter	Vapour-wall friction	Interfacial friction	Vapour-wall heat transfer	Vapour-wall heat flux	Bubbles raise velocity
Estimated θ_h	0.12	0.07	0.04	0.65	0.21
Estimated p_h	2	2	1.93	1.85	2

The kriging model has detected small irregularities of the PCT surface, indicated by estimated values of p_h slightly inferior to 2, for input variables "Initial power", "Vapour-wall heat transfer", and "Vapour-wall heat flux". All estimated values of p_h reveal a smooth kriged surface and a quite linear physical phenomenon.

The model adequacy is checked by cross validation with 221 points test sample calculated at random. We observe on Figure 3 that the points are well distributed around the first bisectrix, which shows that there is no prediction bias at all, except for one outlier (circled) very poorly forecasted by over than 230°C.

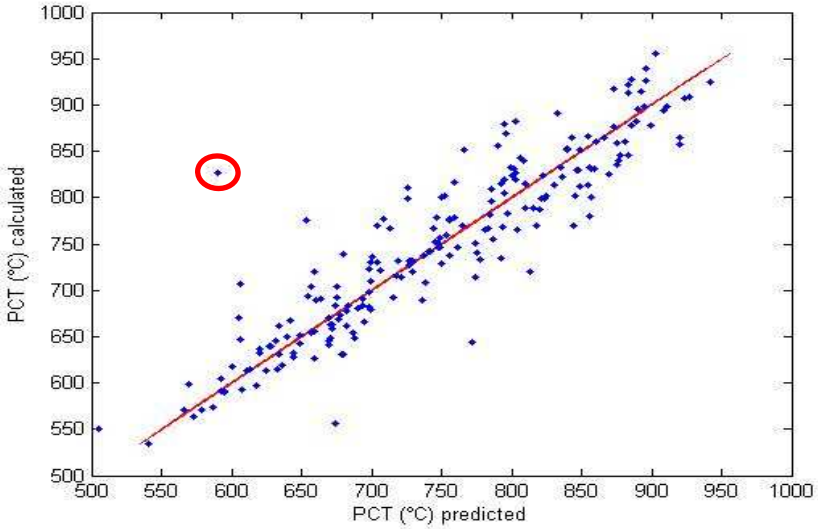

Figure 3. ***Comparison of the simulator outputs and the predictions from the kriging model***

3.2 Sensitivity analysis

The response surface constructed by kriging can be used to identify and to classify the most important parameters and visualize their effects. We present here results of the sensitivity analysis of the kriged surface using coefficients in Table II. Numerical experiments have been made repeating all indices computations 2 times, with N = 400,000 Monte-Carlo iterations. Mean of these 2 estimations are presented in Table III and Table IV.

Table III. Sobol' Indices (First order) for each input parameter

Input Parameter	UO_2 conductivity	Vapour-wall heat flux	UO_2 specific heat	Gap size	Vapour-wall heat transfert	Initial power
Main effect S_i	36.2%	16.1%	14.6%	12.7%	4.6%	2.8%

Input Parameter	Bubbles raise velocity	Vapour-wall friction	Interfacial friction	Residual power	Film boiling
Main effect S_i	2.0%	1.9%	1.6%	1.1%	0.5%

Table IV. Sobol' Indices (Second order) for larger interactions

Input Parameter	UO_2 specific heat / Vapour-wall heat flux	Bubbles raise velocity / Vapour-wall heat flux	UO_2 conductivity / Vapour-wall heat flux	Initial power / Vapour-wall friction
Interaction S_{ij}	1.5%	0.9%	0.7%	0.3%

We can visualize these main effects on Figure 4 which are obtained by averaging the predicted values of a given parameter over all other parameters. It shows a parabolic shape for both parameters "Initial power" and "Vapour-wall heat flux", and near-linear shape for all others. The approach of "scatter plots" is undoubtedly the simplest sensitivity analysis technique, consists of generating plots of the points (input parameter; kriged response), and confirms the last results of sensitivity analysis. We present on Figure 5 the scatter plots (100,000 points) for parameters "Initial power" and "Vapour-wall heat flux" and we note the large dispersion especially for the "Initial power". However, the calculated PCT by Cathare have the same tendency as the calculated PCT by the surrogate model and are bounded by them. It is another mean to check the good accuracy of the kriged response surface.

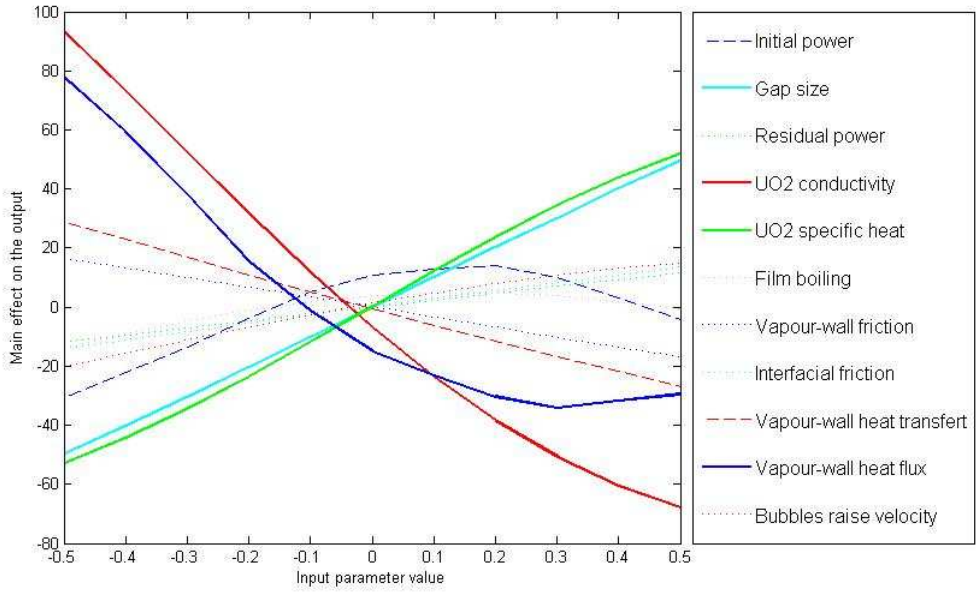

Figure 4. ***Estimated main efftect (PCT's variation (°C)) for each parameter with normalized values in [-0.5; 0.5]***

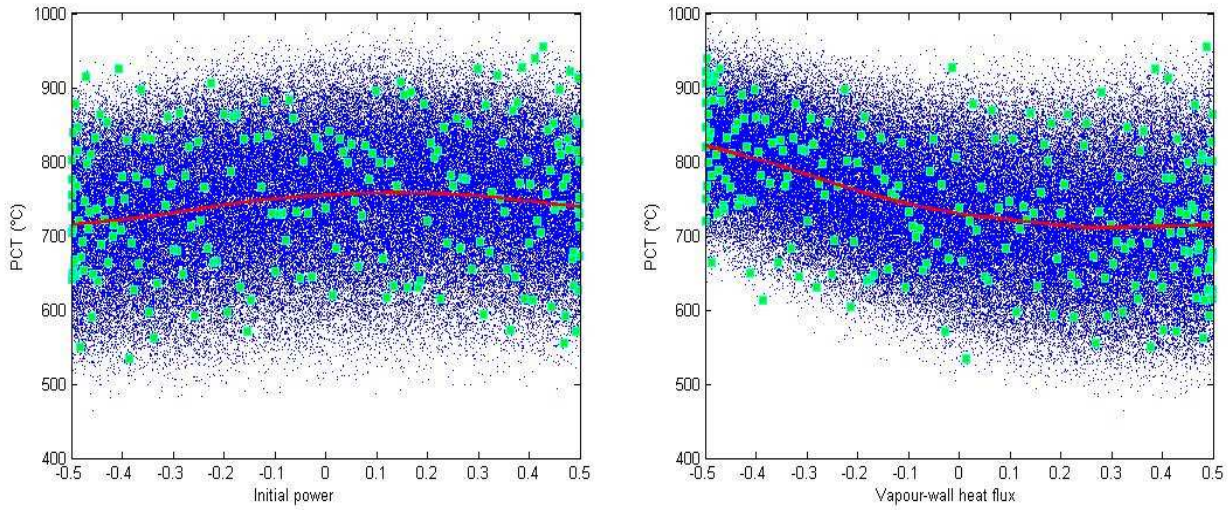

Figure 5. ***Scatter plots for "Initial power" and "Vapour-wall heat flux" with normalized values in [-0.5; 0.5]***
Blue: 100,000 Monte Carlo calculations; Green: 221 LHS points

Multidimensional analysis allows us to conclude that the first PCT is sensitive essentially to input parameters "UO_2 conductivity", "Vapour-wall heat flux", "UO_2 specific heat", and "Gap size". The fraction of output variance explained by the first order indices of those 4 parameters is about 80%. These results are in agreement with the experts judgements and can lead us to think that this methodology could be applied to a real nuclear power plants.

4 CONCLUSIONS

We presented the kriging methodology for the construction of response surfaces, and applied it to the modelling of the Peak Cladding Temperature. It turns out that the kriging technique leads to accurate results in our case study. The principal explanation is that kriging is very flexible, and can handle situations where the PCT surface is smooth in one direction, and irregular in another. We showed a new methodology never used until now of global sensitivity analysis applied to the nuclear application. We coupled the Sobol' approach with a kriged response surface, to quantify the influence of each uncertain input parameter on the response variability of the numerical model.

In the case of LOFT L2-5, this methodology allowed us to classify and quantify the main input parameters which are the "UO_2 conductivity", the "Vapour-wall heat flux", the"UO_2 specific heat", and the "Gap size" of the fuel. These results are in agreement with the experts judgements and can let us think that this methodology could be applied to real nuclear power plant calculations.

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