Comparison of global sensitivity analysis methods – Application to fuel behavior modeling

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HIGHLIGHTS

• Several global sensitivity analysis methods are compared.
• The methods’ applicability to nuclear fuel performance simulations is assessed.
• The implications of large input uncertainties and complex models are discussed.
• Alternative strategies to perform sensitivity analyses are proposed.

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ABSTRACT

Fuel performance codes have two characteristics that make their sensitivity analysis challenging: large uncertainties in input parameters and complex, non-linear and non-additive structure of the models. The complex structure of the code leads to interactions between inputs that show as cross terms in the sensitivity analysis. Due to the large uncertainties of the inputs these interactions are significant, sometimes even dominating the sensitivity analysis. For the same reason, standard linearization techniques do not usually perform well in the analysis of fuel performance codes. More sophisticated methods are typically needed in the analysis. To this end, we compare the performance of several sensitivity analysis methods in the analysis of a steady state FRAPCON simulation. The comparison of importance rankings obtained with the various methods shows that even the simplest methods can be sufficient for the analysis of fuel maximum temperature. However, the analysis of the gap conductance requires more powerful methods that take into account the interactions of the inputs. In some cases, moment-independent methods are needed. We also investigate the computational cost of the various methods and present recommendations as to which methods to use in the analysis.

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1. Introduction

Light water reactor fuel performance codes model the behavior of the fuel rod under irradiation, either in the steady state or in transient conditions. The purpose of the modeling is to provide understanding about how the thermal, mechanical and materials properties interact and how the rod responds as a whole to the boundary conditions imposed by the environment. An important aspect of the analyses is to support the rod design and safe operation, so that the rod cladding remains intact and various safety margins are respected. In addition to the usual difficulty of representing a complex system with soluble mathematical models, there are also large uncertainties in many of the system and model parameters. Therefore sensitivity analyses are often coupled with uncertainty analyses, which take into account the uncertainties in the code input, and produce an estimate of the uncertainty of the calculated result. To take the analysis one step further, one may ask how to reduce the uncertainty of the results, or which of the code inputs is responsible for the uncertainty of the result. These questions can be addressed by sensitivity analysis.

The goal of a sensitivity analysis is to find the most influential input parameter to the computed model output. The method chosen for the sensitivity analysis depends on the computational cost of the model, the number of inputs to be considered, and the specific question to be answered by the analysis. Although adjoint-based methods have been implemented into fuel performance codes in the past (Christensen et al., 1981; Wilderman and Was, 1984), the more generic, sampling-based methods are typically used nowadays. Of these, computationally the most inexpensive method is the one-at-a-time (OAT) method, where each parameter is
varied independently while keeping the others fixed (Geelhoed et al., 2009; Sagrero and Herranz, 2013). Although often used due to its simplicity, the method suffers from poor coverage of the parameter space and from lack of control over the quality of the analysis (Saltelli et al., 2010). For a typical fuel performance code, such as FRAPCON (Geelhoed et al., 2011a,b), the computational time per run is of the order of seconds or minutes. Therefore using Monte Carlo based sensitivity analysis methods is entirely feasible. They have been adopted in many studies to perform global sensitivity analyses (Glaeser, 2008; Boulore et al., 2012; Ikonen and Tulkki, 2014; Pastore et al., 2015). Global sensitivity analysis methods have the advantage of exploring the whole parameter space (hence the term global), and in general can be used to identify properties of very complex models. It should be mentioned that in addition to Monte Carlo based evaluation, global sensitivity analysis can also be performed with computationally more lenient methods (Sudret, 2008).

In this work, we study the practical aspects of using some of the most common global Monte Carlo based sensitivity analysis methods. We apply variance based methods, including the Pearson correlation analysis (Draper and Smith, 1998), and the Sobol’ variance decomposition (Sobol’, 1993). These methods are based on estimating the influence of a given input on the output variance. A closely related method is the elementary effects method (Morris, 1991), which is the global extension of the OAT method. In certain cases it is possible that the variance or other moments of the probability distribution is not a good measure of uncertainty. Then, moment-independent methods can be used. In this work, we employ the density-based Borgonovo δ measure (Borgonovo, 2007), for which an efficient estimation method was recently introduced by Pilschke et al. (2013).

Another consideration when choosing the method is the specific question posed to the analysis. Questions such as “If we could eliminate the uncertainty of one input parameter, which one should we choose in order to reduce the variance of the output as much as possible?” and “Which of the input parameters are so non-influential that they can be fixed?” define the setting of the sensitivity analysis (Saltelli and Saisana, 2007; Saltelli et al., 2008). The first one corresponds to factor prioritization (FP) and the second one to factor fixing (FF) setting. In the FP setting, a good starting point is to determine the main (first order) effect of an input parameter. Higher-order analysis is needed in models with dominating interaction terms (uncertainties in the output that only arise as a result of changing more than one variable simultaneously). Also in the FF setting one has to consider the interactions between different inputs. These can be quantified, for example, by the total effect sensitivity index \( T_i \), the elementary effects method, or in part by the Borgonovo δ measure, discussed in Section 2.

For a fuel performance code, the role of interactions in the model can be significant (Ikonen and Tulkki, 2014). This is because of two characteristics of fuel performance codes: large uncertainties in input parameters and complex, non-linear and non-additive structure of the models. A famous example of the latter is the gap conductance, which couples together the thermal, mechanical and microstructural (e.g., fission gas release) models in the fuel performance code. The intertwined structure of the code leads to interactions between inputs that show as cross terms in the sensitivity analysis. Due to the large uncertainties of the inputs these interactions are significant, sometimes even dominating the sensitivity analysis. For the same reason, standard linearization techniques do not usually perform well in the analysis of fuel performance codes.

A thorough sensitivity analysis of a fuel performance code requires methods that can cope with the large uncertainties and interactions. On the other hand, the simplicity and computational ease of the OAT method is very appealing. In this work, we attempt to address the choice between different methods by comparing their performance in the sensitivity analysis of a steady state scenario modeled with the FRAPCON-3.4 code. In our analysis we focus on the maximum fuel temperature and the gap conductance computed for a mid-burnup (22 MWd/kgU) PWR rod. The latter is particularly challenging to analyze and showcases the potential caveats of the simple methods. We also briefly study the convergence and required computational effort of the methods.

2. Analysis methods

2.1. One-at-a-time (OAT) analysis

Arguably the simplest sensitivity analysis strategy is to vary one model input parameter at a time while keeping the others fixed. Typically such a one-at-a-time (OAT) sampling is done around the nominal (most probable, or best estimate) values of the input parameters. It is possible to choose the sampling points in many ways, but one of the most common ones is to choose the extreme values of the distribution (Sagrero and Herranz, 2013). Another typical way would be to evaluate the effect of infinitesimal changes to the inputs by choosing a very small deviation from the nominal value. However, in the case of a fuel performance code, where we do not expect the model to linearize effectively and where the uncertainties are large, we choose to sample the parameters at their extreme values. One could of course increase the number of points to sample intermediate values of the parameter (Pastore et al., 2015). While this increases the likelihood of catching non-monotonic effects of the input parameters, it also quickly increases the number of required function evaluations, and is unlikely to cover the parameter space efficiently (Saltelli and Annoni, 2010).

The change in the model output is evaluated at all the sampled points, and the input causing the largest change in the output is given the highest rank in the sensitivity analysis. In this work, we define the OAT sensitivity measure for input \( X_i \) as

\[
OAT_i = \frac{\max_{\Delta X_i} f(X + \Delta_i) - f(X)}{\sum_i (\max_{\Delta X_i} f(X + \Delta_i) - f(X))},
\]

where \( X \) is the vector of the nominal values of the inputs, and \( \Delta_i \) is a vector of zeros, except for its \( i \)th element \( \Delta_i^{(i)} \), which is chosen so that \( X_i + \Delta_i^{(i)} \) gives the extrema of the distribution of \( X_i \). The maximum is taken over these two extrema. The function \( f \) represents one of the outputs of the computer code. The denominator serves to normalize the measure so that it can be easily compared to the global sensitivity measures discussed below, which are normalized between 0 and 1 by construction. The normalization has no effect on the parameter ranking.

The computational cost of the method is very small, as the number of required simulation runs is only \( 2k + 1 \), where \( k \) is the number of inputs.

2.2. Global sensitivity analysis

The goal of global sensitivity analysis is to characterize the dependence of the model output on its inputs in the whole input parameter space. Usually the analysis involves some kind of Monte Carlo sampling of the inputs, either by pseudo random sampling or by quasi random sampling. In quasi random sampling, the sample points are chosen in a way that avoids clusters and results in more effective sampling and faster convergence. In this work, the Sobol’ quasi random sequence (Sobol’, 1967) is used to generate the sample points. The variables \( U_i \) generated by the Sobol’ sequence uniformly partition the unit interval \( (0,1) \). The inverse cumulative distribution function (ICDF) method is used to map them to the actual input variables \( X_i \) according to \( X_i = P_i^{-1}(U_i) \), where \( P_i \)
is the CDF of the input $X_i$. The error estimates for the correlation coefficients and sensitivity indices (see below) are calculated by the bootstrap method (Efron, 1979) over at least one hundred bootstrap samples.

2.2.1. Pearson correlation analysis

The simplest global sensitivity analysis of a model is the calculation of linear correlation between an input $X_i$ and the output $f(X_i)$ from (quasi) randomly sampled data (Saltelli et al., 2008). In practice this is done by calculating the Pearson correlation coefficient $R_i$ (Draper and Smith, 1998). The square $R^2_i$ of the Pearson coefficient also gives the portion of the output variance attributable to input $X_i$, and it can be used as a normalized sensitivity measure,

$$ R^2_i = \frac{\text{cov}(X_i, f(X))^2}{V(X_i)V(f(X))} \tag{2} $$

where $V(\cdot)$ denotes the variance and $\text{cov}(\cdot, \cdot)$ the covariance. For uncorrelated inputs, $R^2_i$ is normalized so that $\sum R^2_i \leq 1$, with the equality exact if the model is linear. The sum also gives the overall degree of determination, so it is easy to control that the sensitivity analysis is comprehensive. If the value of the sum remains significantly below unity, the model contains nonlinearities and interactions that can only be analyzed with higher order methods. The ability to check the quality of the sensitivity analysis a posteriori is an important advantage of the Pearson correlation analysis over the OAT methods.

The computational cost of the method is relatively low and (almost) independent of the number of inputs. The number of model runs required for reasonable statistical accuracy depends on the nature of the model, but is typically at least of the order of $N \approx 100$ (Saltelli et al., 2008).

2.2.2. Variance decomposition analysis

A model such as a fuel performance code that has significant interactions between input parameters can be analyzed only incompletely with linear correlation methods. A simple rank transform of the data (for example, the Spearman correlation method) is not sufficient to analyze a fuel performance model comprehensively (Ikonen and Tulkki, 2014). A method that can extract information about the interactions is necessary. One such method is the Sobol’ variance decomposition analysis (Sobol’, 1993).

In the variance decomposition method, the idea is to express the variance $V(f(X))$ of the output as a finite sum of terms of increasing order. Each of these terms represents the contribution of one input variable to the output variance (first order terms) or the variance due to interactions of several variables (higher order terms). For uncorrelated variables, this decomposition is unique (Sobol’, 1993). The Sobol’ sensitivity indices are then defined as these partial variances normalized by the output variance. For example, the first order effect of input $X_i$ is defined as

$$ S_i = \frac{V(E(f(X)|X_i))}{V(f(X))} \tag{3} $$

where $E(f(X)|X_i)$ is the conditional expectation value of $f(X)$ with a fixed value of the input $X_i$. The measure $S_i$ is very similar to $R^2_i$, the difference being that the latter is based on linear regression on the data. However, both measure the portion of output variance that can be directly traced back to the uncertainty in the value of $X_i$. The index $S_i$ is also normalized so that $\sum S_i \leq 1$, with the equality becoming exact if the model is additive (has no interactions).

The analysis of model interactions can be done by computing the higher order terms in the variance decomposition. For computational reasons one typically only analyzes the first and possibly the second order terms, and the so-called total effect index, $T_i$. The index $T_i$ describes the combined effect of the $i$th variable on the output including the first order effect and all the higher order interaction terms between the variable $X_i$ and the other variables, up to the term describing the interactions of all the $k$ inputs of the model. The formal definition for the total effect is

$$ T_i = \frac{E(V(f(X)|X_{-i}))}{V(f(X))} \tag{4} $$

where $V(f(X)|X_{-i})$ denotes the output variance conditional to fixing all the variables except $X_i$. Since the interaction terms are included in the total effects of more than one variable (for example, the interaction between variables $X_i$ and $X_j$ is included in both $T_i$ and $T_j$), the sum of the total effects is not normalized to unity. In fact, $\sum T_i \geq 1$. The equality becomes exact if there are no overlapping terms in the total effects of different inputs (that is, the model has no interactions).

The calculation of the higher order terms can be done efficiently by Monte Carlo integrals for the first order, second order and total effect indices (Saltelli, 2002; Glen and Isaacs, 2012; Ikonen and Tulkki, 2014). Here one uses a special sampling design to estimate the indices (for the details of the numerical implementation used in this work, we refer the reader to Section 3.4.3 of Ikonen and Tulkki (2014), and the work of Glen and Isaacs (2012)). To evaluate the conditional expectations and variances in Eqs. (3) and (4), the design reduces the required computational effort from exponential in $k$ (the number of inputs) to linear in $k$ (Saltelli et al., 2008). Compared to the correlation coefficient analysis, for which the computational cost does not inherently depend on $k$, even the linear scaling remains a limitation for models with tens of uncertain inputs. The required number of model runs is $N(2k + 2)$, where $N$ depends on the desired accuracy, but is typically at least of the order of $N \approx 100$.

2.2.3. Elementary effects method

The elementary effects method is an extension of the OAT method first introduced by Morris (1991). The method consists of sampling the individual effects of inputs to the output by varying the value of one input at a time. In contrast to the OAT method, this sampling is done several times for each input, with the reference point sampled randomly from the whole input space. The implementation can be done in several ways, but a practical option is to use the same radial sampling design as for the variance decomposition analysis (Campolongo et al., 2011). The elementary effect of the $i$th input at the $n$th reference point is

$$ EE_i^n = \frac{f(X_i^n) - f(X_i^n + \Delta_i^n)}{U_i - U_i'}, \tag{5} $$

where $\Delta_i^n$ is defined similarly to the OAT method as a vector of zeros except for the $i$th element, which is $\Delta_i^{(i)} = X_i - X_i'$. Here the point $X_i'$ is sampled independently from the probability distribution of $X_i$ according to the radial design described by Campolongo et al. (2011). In the elementary effects method the inputs are assumed uniformly distributed between (0, 1). Hence, in denominator in Eq. (5) uses the original uniformly distributed variables $U_i$ and $U_i'$ (cf. Section 2.2) corresponding to $X_i$ and $X_i'$ respectively.

From the elementary effects one then defines the importance measures corresponding to the mean ($\mu$), mean of the absolute values ($\mu^*$), and the variance ($\sigma^2$):

$$ \mu_i = \frac{1}{N} \sum_{n=1}^{N} EE_i^n, \tag{6} $$

$$ \mu_i^* = \frac{1}{N} \sum_{n=1}^{N} |EE_i^n|, \tag{7} $$
The elementary effects method is often used as a screening method to reduce the number of inputs. This is because although the computational cost per sample point is similar to the variance decomposition method (proportional to $N(k+1)$), the elementary effects method typically converges faster and thus requires smaller $N$. The measures $\mu_i$, $\mu^*$, and $\sigma^2$ can be used together to extract information about the linearity and additivity of the model. However, if a somewhat simpler analysis is desired, it is often recommended to just use the measure $\mu^*$ (Saltelli et al., 2008; Campolongo et al., 2007). This is the approach we adopt in this work. In addition, to facilitate comparison with the other methods, we normalize the measure similarly to the OAT method so that we will be looking at the quantity $\mu_i^*/\sum \mu_i^*$. The normalization does not affect the ranking of the inputs.

2.2.4. Moment-independent measures

Sometimes the output of a model may have a probability distribution that is difficult to characterize using just the moments of the distribution. For example, the gap conductance calculated by a fuel performance code may have a bimodal distribution, each peak corresponding either to the open gap or the closed gap state. In this case variance-based measures such as the Sobol’ indices and the Pearson correlation coefficient may be inadequate. In such situations it is possible to use moment-independent measures that take into account the changes in the whole probability distribution, not just the variance. One such measure is the $\delta$ measure, introduced by Borgonovo (2007).

The Borgonovo $\delta$ measure calculates the expected shift (difference) in the probability density function of the output $P(x)$ when the value of the input $X_i$ is fixed. The shift is defined as $s(X_i) = \int [P(x|y) - P(x|y)]dy$, where $y = f(x)$ is the value of output for a given realization $x$ of the inputs (see, e.g., Borgonovo (2007) for a graphical interpretation of $s(X_i)$). The $\delta$ measure for the $i$:th input is then

$$\delta_i = \frac{1}{2} E_X[s(X_i)],$$

where $E_X[s(X_i)]$ stands for the expectation value of $s(X_i)$ over the probability distribution of $X_i$.

The estimation of $\delta$ by brute force involves a double integral (first one in $s(X_i)$ and then another to estimate the expectation value of $s$) and is very demanding computationally. Recently Plischke et al. (2013) used a kernel-density estimator to calculate $\delta_i$ from a simple random sample. Kernel-smoothing of the data makes the estimation of $\delta$ much less computationally demanding and, perhaps more importantly, allows one to use the same sample set as for the Pearson correlation coefficient. The bias due to finite sample size for low-importance inputs can be reduced by filtering with a Kolmogorov–Smirnov test (Pischke et al., 2013). In this work, we use a diffusion kernel estimator for calculation of $\delta$ implemented in Matlab by the developer of the method (Plischke, 2015).

3. Fuel performance model and the simulated scenario

To illustrate the capabilities of the sensitivity analysis methods in practice, we study the propagation of uncertainties under steady-state irradiation with the FRAPCON-3.4 fuel performance code (Geelhoed et al., 2011a,b). FRAPCON is a deterministic fuel performance code that calculates the steady-state response of light-water reactor fuel rods during long-term burn-up. Boundary conditions such as the power history and the coolant properties, in addition to the rod fabrication parameters, are supplied as input. Additionally, several model parameters can be re-defined in the input both in the official version of the Pacific Northwest National Laboratory (PNNL) and in the version modified at VTT Technical Research Centre of Finland. The output of the code comprises several observables. A thorough analysis of the most important ones has been done previously with the Sobol’ variance decomposition method (Ikonen and Tulkki, 2014). In this work, we focus only on the pellet centerline temperature, and the gap conductance. Based on the previous work, we expect the gap conductance to be more difficult to analyze. The intuitive reason for this is that in solving the equations defining the gap conductance, the fuel performance code takes into account both the thermal and mechanical behavior models, which essentially leads to cross terms in the sensitivity analysis that may be difficult to pin-point. The centerline temperature, on the other hand, is much more straightforward to analyze, and even simple methods should be quite effective.

The analyzed scenario is a hypothetical steady-state irradiation of a UO$_2$ fuel rod in the Three Mile Island 1 (TMI-1) PWR reactor. The scenario is designed to bring the fuel rod to a relatively high burn-up of 50–60 MWd/kgU (depending on the input values), using a simplified power history, where the average linear heat rate is 23.39 kW/m from the beginning of the irradiation until 550 days, 19.69 kW/m until 1200 days and 15.0 kW/m until the end of irradiation at 1800 days. The axial power profile is given in Table 1.

<table>
<thead>
<tr>
<th>Position (mm)</th>
<th>0.0</th>
<th>304.8</th>
<th>609.6</th>
<th>914.4</th>
<th>2743.2</th>
<th>3048.0</th>
<th>3352.8</th>
<th>3657.6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative power</td>
<td>0.63</td>
<td>0.83</td>
<td>1.03</td>
<td>1.08</td>
<td>1.08</td>
<td>1.03</td>
<td>0.83</td>
<td>0.63</td>
</tr>
</tbody>
</table>

The variability of the fuel parameters is accounted for by assuming different input values, ranging from 0.5 to 1.5, in the calculation of the expected output

$$\sigma_i^2 = \frac{1}{N-1} \sum_{n=1}^{N} (E[X_i^n] - \mu_i)^2.$$
Table 2
The best estimate values of input parameters and their uncertainties used in the analyzed scenario. If no uncertainties are indicated, the input was not varied. For the FRAPCON correlations and the power history (the bottom half of the table) only uncertainties are shown, since the best estimate value is a function of several variables or changes with time.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Clad outer diameter</td>
<td>(10.92 ± 0.06) mm</td>
</tr>
<tr>
<td>Clad thickness</td>
<td>(0.673 ± 0.025) mm</td>
</tr>
<tr>
<td>Pellet outer diameter</td>
<td>(9.40 ± 0.02) mm</td>
</tr>
<tr>
<td>Total fuel height</td>
<td>3657.6 mm</td>
</tr>
<tr>
<td>Fuel pellet height</td>
<td>11.43 mm</td>
</tr>
<tr>
<td>Fuel enrichment (atom.%)</td>
<td>(4.85 ± 0.003)%</td>
</tr>
<tr>
<td>Density (% of theoretical)</td>
<td>(93.8 ± 1.6)%</td>
</tr>
<tr>
<td>Clad type</td>
<td>Zr-4</td>
</tr>
<tr>
<td>Fill gas type</td>
<td>Helium</td>
</tr>
<tr>
<td>Fill gas pressure</td>
<td>1207 kPa</td>
</tr>
<tr>
<td>Fuel rod pitch</td>
<td>14.43 mm</td>
</tr>
<tr>
<td>Coolant pressure</td>
<td>(15.51 ± 0.31) MPa</td>
</tr>
<tr>
<td>Coolant inlet temperature</td>
<td>(561 ± 3) K</td>
</tr>
<tr>
<td>Coolant mass flux</td>
<td>(3460 ± 69) kg/(m²s)</td>
</tr>
<tr>
<td>Fuel thermal conductivity</td>
<td>±10%</td>
</tr>
<tr>
<td>Fuel thermal expansion</td>
<td>±15%</td>
</tr>
<tr>
<td>FGR diffusion coefficient</td>
<td>±200%/−67%</td>
</tr>
<tr>
<td>Fuel swelling</td>
<td>±20%</td>
</tr>
<tr>
<td>Clad creep</td>
<td>±30%</td>
</tr>
<tr>
<td>Clad axial growth</td>
<td>±50%</td>
</tr>
<tr>
<td>Clad corrosion</td>
<td>±40%</td>
</tr>
<tr>
<td>Clad H concentration</td>
<td>±80 ppm</td>
</tr>
<tr>
<td>Clad thermal conductivity</td>
<td>±5 W/mK</td>
</tr>
<tr>
<td>Clad thermal expansion</td>
<td>±30%</td>
</tr>
<tr>
<td>Gas thermal conductivity</td>
<td>±0.02 W/mK</td>
</tr>
<tr>
<td>Coolant heat transfer</td>
<td>±5%</td>
</tr>
<tr>
<td>Linear power</td>
<td>±5%</td>
</tr>
</tbody>
</table>

4. Results and discussion

4.1. Uncertainty analysis

Before going into the sensitivity analysis, we take a look at the results from the uncertainty analysis of the scenario described in Section 3. The scenario was simulated with VTT-modified FRAPCON-3.4 on a Linux cluster. The input parameters were sampled independently from their respective probability distributions, with a sample size of $N = 50,000$. In addition, for the Sobol’ sensitivity indices and elementary effects, an additional 22 sample sets were generated, bringing to total number of simulation runs to $1.15 \times 10^6$, which took approximately 20 CPU-days on the Linux cluster. However, as will be shown by the convergence analysis in Section 4.4, in most cases satisfactory accuracy can be achieved with much smaller $N$.

From the calculated results, we choose just two for further analysis: the maximum fuel temperature $T_{\text{max}}$ and the gap conductance $h_{\text{gap}}$ at the central axial node, both evaluated at the burnup of approximately 22 MWd/kgU, where the gap can be either open or closed, depending on the values of the inputs (Ikonen and Tulkki, 2014). The evolution of the mean values and uncertainties of $T_{\text{max}}$ and $h_{\text{gap}}$ with increasing burnup are shown in Figs. 1 and 2. The sharp changes in the graphs correspond to the drops in linear power occurring at approximately 21 MWd/kgU and 40 MWd/kgU. The probability distributions of $T_{\text{max}}$ and $h_{\text{gap}}$ at 22 MWd/kgU are also shown in the insets.

Already from the probability distributions of $T_{\text{max}}$ and $h_{\text{gap}}$, it is possible to make some deductions. The distribution of $T_{\text{max}}$ is almost Gaussian. Therefore it is likely that the model that produces the distribution of $T_{\text{max}}$ from the (almost Gaussian) input distributions is quite simple. On the contrary, the distribution of $h_{\text{gap}}$ is very complex, having a bimodal main part, with each peak corresponding to either the closed gap or open gap state, and a long tail towards zero. It is not likely that such a distribution could be produced by any simple model, so we may expect to find significant nonlinear and interaction terms. In fact, the behavior is typical of a model where crossing a certain threshold (gap closure) abruptly changes the behavior of the system (switching from conduction across gas to conduction through points of contact). The bimodality also suggests that moment-independent methods (e.g., $\delta$) may be needed to analyze some inputs. For both $T_{\text{max}}$ and $h_{\text{gap}}$ the uncertainty in their value is high.

4.2. Sensitivity analysis

From the same set of simulation runs that were used in the uncertainty analysis, the sensitivity measures described in Section 2 were estimated. The full set of $N = 50,000$ simulations were used in the estimation; the convergence of the results and the required number of samples is discussed in Section 4.4. It should be noted that the results discussed below apply only at the burnup of 22 MWd/kgU in the specified scenario. For the burnup-dependence of the sensitivity indices, the reader is referred to the study of Ikonen and Tulkki (2014).

The results for the maximum temperature are shown in Fig. 3 and for the gap conductance in Fig. 4. In the case of the maximum temperature, the results between the different methods are very similar. All methods rank the fuel thermal conductivity as the most influential, followed by the average linear heat rate (ALHR). The rest of the inputs are almost negligible. It is important to note that the
correlation is ranked quite low, except for the $\delta$ measure, which gives it the highest rank. This detail will be discussed below.

For the gap conductance, one typically finds that $R^2 \neq S_i$ and $S_i \neq T_i$. This means that the underlying model is non-linear and non-additive with respect to the gap conductance. In such a case, full model analysis requires using higher order and possibly moment-independent methods. In particular, the simple correlation coefficient analysis will only explain a certain fraction of the variance. In this case, $\sum R^2_i \approx 0.53$, meaning that almost half of the variance is unaccounted for. Analysis of the rank correlation coefficient or the first order Sobol’ terms do not work much better, as discussed by Ikonen and Tulikki (2014).

The bimodal probability distribution of the gap conductance (see inset of Fig. 2) can make certain inputs very difficult to analyze. This is shown in the difference in the ranking of the gas thermal conductivity in Fig. 4, where the $\delta$ measure gives a value of 0.48 and the other methods values close to 0.05. The reason is that the effect of the gap conductivity on the probability distribution is to shift both of the peaks by the same amount to the left (low conductivity) or to the right (high conductivity). This shift is captured in full by the $\delta$ measure. However, the variance of the distribution remains almost unchanged under such a shift, which makes variance based methods such as Sobol’ variance decomposition or correlation coefficients ineffective.

### 4.3. Ranking comparison

It is clear that comprehensive knowledge of the model’s sensitivities can only be achieved by using higher order or moment-independent methods. However, it is often practically desirable to use simpler methods for initial screening of inputs or even for the final analysis. It is therefore a relevant question to ask if one can achieve the same ranking of the inputs by only using the simple methods. For this purpose, we rank the inputs in the order of the estimated sensitivity measures and compare the rankings between the different methods.

Instead of directly comparing the ranks, we calculate a so-called Savage score for each of the inputs. The Savage scores are defined as (Savage, 1956)

$$SS_i = \sum_{j=r_i}^{k} \frac{1}{j},$$

(10)

where $k$ is the number of inputs and $r_i$ is the rank of the $i$th input. The input with the highest value of the sensitivity measure has a rank of 1. The advantage of the Savage scores is that the least influential inputs receive very similar scores, and thus the dominant inputs have more weight in the comparison.

Table 3 shows the Pearson correlation coefficients calculated from the Savage scores between the various methods. The self-correlation is by definition 1 (any method gives the same input ranking as itself when using the same sample set), and values close to 1 indicate differences in the low-ranking inputs only. It can be seen that the largest differences are between the derivative-based (OAT and $\mu^*$) and the variance-based ($R^2$, $S$ and $T$) methods, but even then the correlation coefficient is larger than 0.96. This means that the rankings are essentially the same with all the methods. This is of course evident in Fig. 3.

For the gap conductance, the comparison is more interesting. The variance-based methods give similar rankings (correlation coefficient larger than 0.94). It is also seen that $\mu^*$ is quite a good proxy for the total effect $T$ (correlation coefficient is larger than 0.95), as suggested by Campolongo et al. (2007). The ranking of the OAT method is quite different from the rest, at most scoring less than 0.85. The most striking fact is however, that the ranking by
the δ measure correlates very weakly with the rest. The reason is that δ is the only method that captures the dependence of the gap conductance on the gas conductivity. None of the other methods can reproduce the same ranking, and in fact typically give a very low rank for the gas conductivity (Table 4).

### 4.4. Numerical convergence and computational cost

In addition to the capability to extract the relevant information from the model, another important aspect of a sensitivity analysis method is its computational cost. We have compared the numerical convergence of the methods by calculating the sensitivity measures with various sample sizes N and sampling the statistical error with the bootstrap method (Efron, 1979). At least 100 bootstrap samples were used. It should be noted that with the sampling design that was used, the elementary effects (μ*) and variance decomposition (S and T) methods have a computational cost (number of model runs) of 2N(k + 1), where k = 21 is the number of inputs in this study. The R² and δ measures require just N model runs for the sample of size N.

To calculate the relative errors we divide the statistical 95% confidence range obtained from the bootstrapped sample of size N with the bootstrap mean calculated from the same sample. This was repeated for sample sizes between N = 32 and N = 32768. The results are shown in Figs. 5–7. The first one (Fig. 5) shows the convergence of the sensitivity measure between the maximum temperature and the fuel thermal conductivity. Overall, the errors are quite small, with the relative error of 0.1 reached for N = 128–512 depending on the method. Evaluated in terms of model runs, the fastest method to converge is R², followed by δ. However, its computational cost is comparable to μ* and, for a smaller number of inputs k, could in fact be slower than all the other methods. Out of μ*, S and T, the fastest to converge is μ*. Somewhat surprisingly, the total effect T converges faster than the first order effect S. It should be noted the convergence of S and T depends greatly on how they are calculated (Saltelli, 2002; Glen and Isaacs, 2012), and it may be possible to further optimize the calculation of S.

In the case of the gap conductance, the situation is very different. Reaching the 0.1 relative error takes several thousand independent samples (see Figs. 6 and 7). In addition, the mean value of the R² measure is not the fastest to converge. For a reasonable sample size (e.g., N ≥ 128), the estimator for δ converges faster than R², as measured by the relative error. It is interesting to note that for the gas conductivity, the convergence of R² is slower than μ*, S and T, even taking into account the sampling design that multiplies their computational effort by 2(k + 1). Overall, the μ* measure converges the fastest in this case. Of course, it may be argued that δ is the only measure that converges to a value that is representative of the gap conductance’s sensitivity to the gas conductivity. The observation of fast convergence of μ* is thus rather moot.
5. Summary

We have evaluated the performance of several sensitivity analysis methods in the context of fuel performance modeling. Fuel performance codes suffer from large uncertainties in their input parameters that, coupled with the complex structure of the models, lead to strong interaction effects. These interactions can make standard linearization approaches ineffective in the sensitivity analysis of a fuel performance code, as shown in the case of the gap conductance. Similarly, methods such as one-at-a-time (OAT) sampling or calculation of correlation coefficients, although simple to use, turn out inadequate. However, the advantage of the Pearson correlation coefficient analysis over the OAT method is that it is possible to check the quality of the analysis a posteriori by computing the explained variance, \( \sum R^2 \). For the OAT method, this is not possible. Of course, if the computational cost of the code is so high that only a few model runs can be afforded, then the OAT method or some of its extensions (Saltelli and Annoni, 2010) may be viable alternatives. Alternatively, surrogate or metamodeling techniques may be attempted (Sudret, 2008; Saltelli et al., 2008; Iooss and Lemaitre, 2015). However, if at least about one hundred model runs can be afforded then a Monte Carlo based global sensitivity analysis method can be directly employed.

Although the global analysis can start with the correlation coefficient analysis, if the explained variance remains low, it is advisable to use methods that can take into account the interactions. For example, the Sobol’ total effect index \( T_i \) or the elementary effects, in particular \( \mu_i^* \), can be analyzed. The Sobol’ variance decomposition can be very effective in fuel performance code analysis (Ikonen and Tuikki, 2014). The drawbacks of the method are the special sampling design that is required to estimate the total effect, and the increased computational effort that is needed to evaluate the sensitivity indices. Compared to the Pearson correlation coefficient analysis, the required computational effort varies, but is typically about a factor of 2\((k+1)\) higher (cf. Figs. 5–7). The elementary effects method is considerably faster, even so that it is a viable alternative for OAT analysis of high computational cost codes. The measure \( \mu_i^* \) is also a good proxy for the total effect \( T_i \).

Sometimes the output probability distribution may significantly deviate from Gaussian. In such cases, it is possible that the variance of the output cannot describe the distribution in a sufficient manner. This is the case of the gap conductance, where using only variance-based measures may lead to overlooking the contribution of the gas conductivity. We show that a moment-independent measure, for example the Borgonovo \( \delta \), can reveal significant contributions overlooked by the variance analysis. By virtue of recent advances, the estimation of the \( \delta \) measure is computationally efficient, and requires no special sampling designs (Plischke et al., 2013; Plischke, 2015).

The present work suggests two strategies for global sensitivity analysis. According to the first, more simple approach, the values of the input parameters are chosen by ordinary random or quasi-random sampling. From the resulting data, the Pearson correlation coefficients \( R \) and the Borgonovo \( \delta \) can be calculated. If the sum of the squared coefficients, \( \sum R^2 \), remains significantly below unity, the Borgonovo \( \delta \) can be used to detect nonlinearities and other effects that elude the linear analysis. To classify the interactions and nonlinearities, it is possible to use also additional methods (Borgonovo and Plischke, 2015), or employ the second strategy. In the second strategy, the input parameters are sampled as required by the Sobol’ variance decomposition method. From the data, elementary effects, Sobol’ indices and the Borgonovo \( \delta \) can be calculated. If the sample size can be made large enough, the calculation of elementary effects can also be omitted. This strategy covers nonlinearities, interactions, and effects not detected in the variance. However, it requires setting up the sampling design and is computationally more intensive. The analyst should also keep in mind the question posed to the sensitivity analysis (i.e., the setting of the analysis) and choose the method so that it can provide an answer to the question (Saltelli et al., 2008; Borgonovo and Plischke, 2015).

The present work is not limited to nuclear fuel performance codes. The central results should be useful in choosing the sensitivity analysis methods for any code with significant input uncertainties and complex structure, including, for example, thermal hydraulics and nuclear system codes. The recommendations follow the best practices of sensitivity analysis set forth in previous literature (see, e.g., Saltelli et al. (2008), Iooss and Lemaitre (2015)). However, the importance of also considering moment-independent measures (Borgonovo and Plischke, 2015) is emphasized.

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