Investigation of Different Sampling and Sensitivity Analysis Methods Applied to a Complex Model for a Final Repository for Radioactive Waste

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Abstract: The performance of different types of sensitivity analysis methods in combination with different sampling methods on the basis of a Performance Assessment model for a repository for Low and Intermediate Level radioactive Waste (LILW) in rock salt has been investigated. This paper provides an insight into the results obtained with the following methods for sensitivity analysis: (i) a graphical method (CSM plot), (ii) a rank regression based method (SRRC) and (iii) a simple first-order SI calculations scheme (EASI). These methods were combined with random and LpTau sampling. The most robust results were obtained using LpTau sampling. The results obtained with CSM and SRRC analysis are fairly comparable. The EASI results, however, assign the dominating role to a parameter that seemed to be of secondary importance according to the results of the two other methods before. In addition, in the early phase below 10^4 years, the EASI results seem to be of low robustness.

Keywords: CSM plot, EASI, rank regression based method (SRRC), LpTau sampling, quasi-random sampling.

1. INTRODUCTION

For the assessment of the long-term safety of a geological repository for radioactive waste, adequate handling of the various uncertainties within the system and the available data is essential. Computational models for the Performance Assessment (PA) of final repositories, especially in a rock salt environment, typically include a number of interacting physical and chemical effects, which leads to a non-linear, non-monotonic and sometimes even virtually non-continuous behavior. A robust and reliable global sensitivity analysis of such models can be a demanding task, which requires a sufficiently high number of runs with a good coverage of the parameter space.

Simple random sampling is often not the best choice, since it tends to developing clusters and gaps in the parameter space. More sophisticated types of sampling techniques for Monte-Carlo methods such as Quasi-Monte-Carlo sampling have been developed to improve convergence and/or accuracy of probabilistic evaluations. Recent literature studies indicate that Quasi-Monte-Carlo sampling schemes can give more robust sensitivity measures with a lower number of simulations than random sequences, as the parameter space is covered more homogeneously.

The most adequate combination of a sampling scheme and a sensitivity analysis method may not only depend on the CPU cost and time of the analysis and the required accuracy but also on the system behavior (degree of linearity and monotonicity, discrete nature), the number of parameters and parameter interaction. This may be in particular important for comprehensive computational models that take account of a variety of different coupled processes. For instance, variance-based methods are recommended for computational models showing a non-linear and non-monotonic system behavior.

In combination with different sampling methods, the performance of different types of sensitivity analysis methods on the basis of a Performance Assessment model for a repository for Low and Intermediate Level radioactive Waste (LILW) in rock salt has been studied. This PA model shows a nearly non-continuous or quasi-discrete behavior as result of the dissolution and nearly sudden failure of the seal in the near field. When this barrier fails, a sudden high release of radionuclides, i.e., a jump in the model output occurs.

This paper provides an insight into the results of the following methods for sensitivity analysis:

- a graphical method (CSM plot),
- a rank-regression-based method (SRRC) and
- a simple first-order SI calculations scheme (EASI).

These methods were combined with random and LpTau sampling. The LpTau scheme belongs to the group of Quasi-Monte-Carlo sampling schemes. Numerous sample sets of different sizes generated by the different sampling schemes were examined.

2. METHODS

2.1. Sampling Techniques

With the random method, the sample values are randomly selected within the parameter space following given probabilistic density functions (pdfs). Random samples typically show some clustering and gaps in the parameter space. The quasi-random LP-Tau sequence (LpTau) belongs to the group of low-discrepancy sequences. It is designed to prevent clustering and gaps of sampling points as much as possible even for fairly small samples by placing the points as homogeneous as possible within the space. The LpTau sequence starts with the generation of Sobol sequences. The Sobol sequences establish successively finer partitions of the [0,1] interval on the base of two and then rearrange the coordinates in each dimension. The generated sample is then transformed to the desired intervals for each parameter. It was found to be a very fast computational algorithm.

2.2. Methods for Sensitivity Analysis

CSM (Contribution to Sample Mean) plots are obtained by sorting the model output values according to increasing values of the considered input parameter and then plotting the total contribution to the mean of the output versus the proportional size of increasing subsets. The more the curve deviates from the diagonal the higher is the sensitivity of the model against the respective parameter. A left-curved progression, normally below the diagonal, means a positive influence (parameter increase → output increase); a right-curved progression, normally above the diagonal, represents a negative influence (parameter increase → output decrease). More details about CSM plots can be obtained from [1,2].

SRRC (Standardized Rank Regression Coefficients) are calculated as the coefficients of a multilinear regression between the input and the output ranks [3]. By the rank transformation the nonlinear, but largely monotonic model is better adapted to linear regression. Positive SRRC values mean a positive influence, negative values a negative influence.

EASI stands for an effective algorithm for estimating sensitivity indices of first order [4]. In contrast to the FAST/EFAST methods, which require specific frequency data for the input parameters, EASI can introduce these into existing sample sets. This is accomplished by sorting and shuffling the values of the different input parameters. The output is arranged according to the input data. The arranged data are then analyzed using the power spectrum of the output as it is done in FAST/EFAST. A big advantage of EASI is that any sampling scheme can be applied, existing samples can be extended and model evaluations can be re-used.

As EASI belongs to the group of variance-based sensitivity analysis methods, changes in the model output are squared in the computation of SI1. For this reason, the direction of influence cannot be found by such methods. Moreover, they tend to overvaluing very high values, especially if the output varies over orders of magnitude. A characteristic of PA models is that a small fraction of output values may be rather high compared to the rest of the values.

3. MODEL AND SOFTWARE

The investigated model consists of three parts, describing the near field, the geosphere and the biosphere. In the near field part it is assumed that the mine openings are filled with brine from the overburden after some time. At that point in time, some short-lived wastes, which are disposed of in one of the openings, start to release contaminants. These are dissolved in the brine and pressed out to the geosphere by the convergence process. In order to protect the longer-lived and more radiotoxic wastes from the brine, the main waste emplacement area is isolated from the rest of the mine by a specific seal, which, however, can be chemically corroded by magnesium. Depending on the magnesium content of the brine and the initial permeability of the seal material, the seal can nearly suddenly fail at some point in time. This leads to a short-lasting decrease, followed by a fast, significant increase of the contaminant release. The decrease is due to the fact that after seal failure it takes some time to fill up the emplacement area, during which the brine outflow from the mine is reduced.

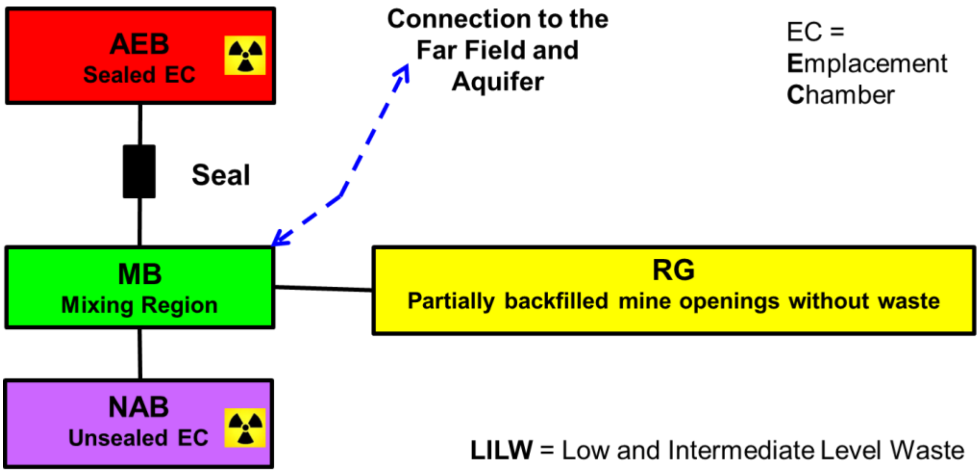
As model output, the annual effective dose to an adult human individual is calculated with the software package RepoTREND [5]. This package contains independent modules for the near field, the far field and the biosphere to calculate the transport of brine and radionuclides through the repository system. The three modules for the near field, the far field and the biosphere are called LOPOS, GeoTREND-POSA and BioTREND, respectively.

All samples were generated using the software package SIMLAB 3.2.6, developed by the Joint Research Centre (JRC) in Ispra (http://simlab.jrc.ec.europa.eu), within the MATLAB environment. The EASI analysis was done using the MATLAB script by [4]. This script can also be downloaded from the JRC website.

4. PERFORMANCE ASSESSMENT (PA) TEST CASE

The model structure of the near field is schematically shown in Figure 1. It consists of two emplacement chambers (EC) with emplaced radioactive waste, one of which is sealed and the other one is not (AEB and NAB, respectively), a mixing region (MB) and the partially backfilled residual mine without waste (RG). The mixing region is connected to both ECs and the residual mine and acts as the interface to the far field.

Figure 1: Illustration of the Near Field Model of the LILW Repository System in Salt



For the probabilistic investigations of the model, in total, 11 parameters, all pertaining to the near field, were varied with adequate probability density functions (pdfs). These parameters, along with their abbreviations, distribution types and ranges, are listed in Table 1.

Table 1. Distributions and Ranges of the Parameters of the PA Model for an LILW Repository in Rock Salt

Parameter	Unit	Description	Distribution Type	Minimum μ(1) Peak(3)	Maximum σ(2)
IniPermSeal	$[m^2]$	Initial Permeability of Dissolving Seal	Normal	$3.23\cdot10^{-21}$ $41.0605^{(1)}$	$6.7\cdot10^{-16}$ $1.9809^{(2)}$
AEBConv	[-]	Factor of Local Convergence Variation in the Sealed Emplacement Chamber	Log Uniform	0.05	5
GasEntryP	[MPa]	Gas Entry Pressure	Uniform	0	2.5
GasCorrPE	[1/yr]	Corrosion Rate of Organics	Log Normal	10^{-7} $-12.6642^{(1)}$	10^{-4} $1.1177^{(2)}$
RefConv	[1/yr]	Reference Convergence Rate	Log Uniform	10^{-5}	10^{-4}
TBrine	[yr]	Brine Intrusion Time	Log Normal	848.4 $8.8857^{(1)}$	61573 $0.6933^{(2)}$
MgBrineSat	[-]	Relative Magnesium Saturation of Brine	Triangular	0 $0.1^{(3)}$	1
RGConv	[-]	Factor of Local Convergence Variation in the Partially Backfilled Mine Openings without Waste	Log Uniform	0.25	2.5
GasCorrFe	[1/yr]	Corrosion Rate of Metal	Log Normal	$4\cdot10^{-5}$ $-6.6728^{(1)}$	$4\cdot10^{-2}$ $1.1177^{(2)}$
AEBGasProd	[-]	Proportion of the Material Involved in Gas Production in the Sealed Emplacement Chamber	Triangular	0.1 $0.8^{(3)}$	1
NABGasProd	[-]	Proportion of the Material Involved in Gas Production in the Unsealed Emplacement Chamber	Triangular	0.1 $0.8^{(3)}$	1

(1) μ value(*)
(2) σ value with quantiles of 0.001 and 0.999(*)
(*) μ and σ values describe mean value and standard deviation of a normal or lognormal distribution
(3) Peak value of the triangular distribution

The seal of the emplacement chamber AEB can dissolve over time. Since the dissolution front progresses linearly through the seal and even a short piece of intact material still has a notable sealing capability, the seal fails nearly suddenly when the front reaches its end. This happens after a specific time, dependent on certain parameters. Therefore, two stages of model behavior need to be considered. As long as the seal is still functioning, the radionuclides are retained to a great extent in the emplacement chamber AEB. After failure of the seal, the radionuclides can be released from the emplacement chamber much quicker and the PA model may consequently bring forth much higher dose values. The transition between both kinds of model behavior, which happens very fast on the considered time scale, is the reason for the quasi non-continuous or quasi-discrete behavior of the LILW model, as it can cause a drastic jump in the model output.

Two parameters have a major influence on the time of seal failure. These are the initial permeability of the seal (IniPermSeal) and the magnesium saturation of the brine (MgBrineSat). Higher values of one or both of these parameters mean faster dissolution and earlier seal failure. Therefore, slight changes of these values can cause considerable jumps of the model output if investigated at a specific point in time, which makes the parameters act like switches. Additionally, the gas entry pressure (GasEntryP) behaves similarly as a switch, since the model behavior essentially changes depending on whether the gas entry pressure is below or above the value of 1.0 MPa. This is the threshold value for release of gas from the top of the sealed emplacement area AEB. This effect can lead to an increase of maximum release by more than one order of magnitude, caused by a very slight increase of GasEntryP.

5. USED SAMPLES

In total, five different samples were generated for the set with 11 parameters using random and LpTau sampling. The four random samples have sizes of 2048, 4096, 8192 and 16384 simulations. Only one LpTau sample with a size of 16384 was generated, which was broken into sets of 2048, 4096, 8192 and 16384. Table 2 lists the samples and sample sizes for each sampling technique.

Table 2. Investigated Numbers of Samples and Sample Sizes Used for the Different Sampling Schemes

Sampling Technique	Number of Samples	Sample Sizes (Number of Simulations)
Random	4	2048, 4096, 8192 and 16384
LpTau	1	

6. RESULTS

For each sampling and analysis method, time-dependent sensitivity measures (SM's) were determined. These are computed from 301 discrete annual dose values distributed over the simulation interval of 10^6 years. For the time-dependent CSM analysis, CSM curves were generated from the annual dose for each parameter at 201 time points and plotted in one figure in different colors. In this way, the time evolution of the curves is visualized. Time points below 10^4 years are not analyzed with the concept of the CSM plot as those do not provide representative CSM curves.

Results of the CSM and SRRC analysis identify the parameters IniPermSeal, AEBConv and TBrine as most important, though TBrine plays a role only in the early phase. Additionally, the parameters GasEntryP, RefConv and GasCorrPE seem to have some importance, at least in specific time phases.

The EASI analysis gives a similar impression, but assigns an outstanding importance to AEBConv. As EASI belongs to the group of variance-based methods, changes in the model output are squared in the computation of first-order sensitivity indices (SI1). This can lead to results significantly different from those obtained by linear methods, especially if the output varies over orders of magnitude. An approach to mitigating possible overvaluation of extreme values by output transformation is presented in [6].

Moreover, unlike regression- or correlation based methods, variance-based methods are unable to determine the direction of influence. This can be seen in particular at the parameters GasEntryP and GasCorrPE, which show a zero-crossing in their SRRC curves and have CSM plots extending over both sides of the diagonal. Obviously, there are opposing influences of the same parameter to the model output, annihilating each other at some point in time. The EASI SI1 curves reach zero at this point and then increase again or show a plateau.

The results obtained with the different sensitivity analysis methods using random sampling show that the deviations between the different sets with the same number of runs are bigger compared to the ones using LpTau sampling. This is revealed in particular by the results of the EASI method.

It seems that the methods investigated in this paper do not provide complete picture of the sensitivity. In another investigation [7] we showed for the same PA model that the parameter MgBrineSat, which appeared to be nearly non-important by itself, has a significant impact on the sensitivities of two other parameters (IniPermSeal, AEBConv). This parameter of indirect importance could only be identified by investigating different sets of parameters.

6.1. CSM plot

In Figure 2, color-coded time dependent CSM plots for all 11 parameters, calculated from a set of 16384 runs with LpTau sampling, are presented. For some of the parameters, the black curves show an extreme deviation, indicating that these parameters play a role mainly in the early phase. This applies in particular for TBrine, but also for IniPermSeal. The parameter GasFeConv has significant curves only for very early times. Disregarding the black curves, the parameter AEBConv shows the most conspicuous diagram with a widely expanded set of curves.

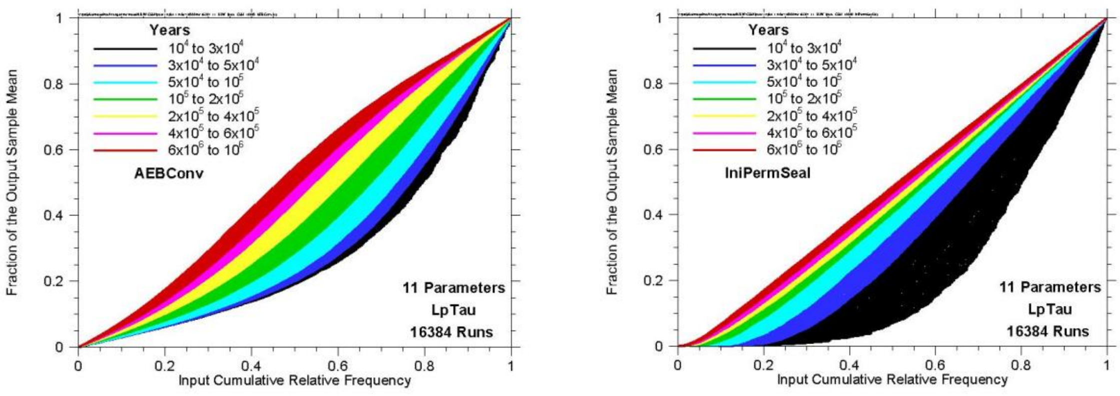
The parameter GasEntryP also produces a wide set of curves, all of which have a sharp bend at 0.4. This is due to the fact that there is a critical value of GasEntryP at which gas release from the emplacement area becomes impossible, which leads to a completely different model behavior. The parameter is distributed in such a way that 40% of the drawn values are below this critical value and 60% above. It is interesting that the CSM curves of GasEntryP expand over both sides of the diagonal, which means that the parameter changes its direction of influence to the model output at some point in time.

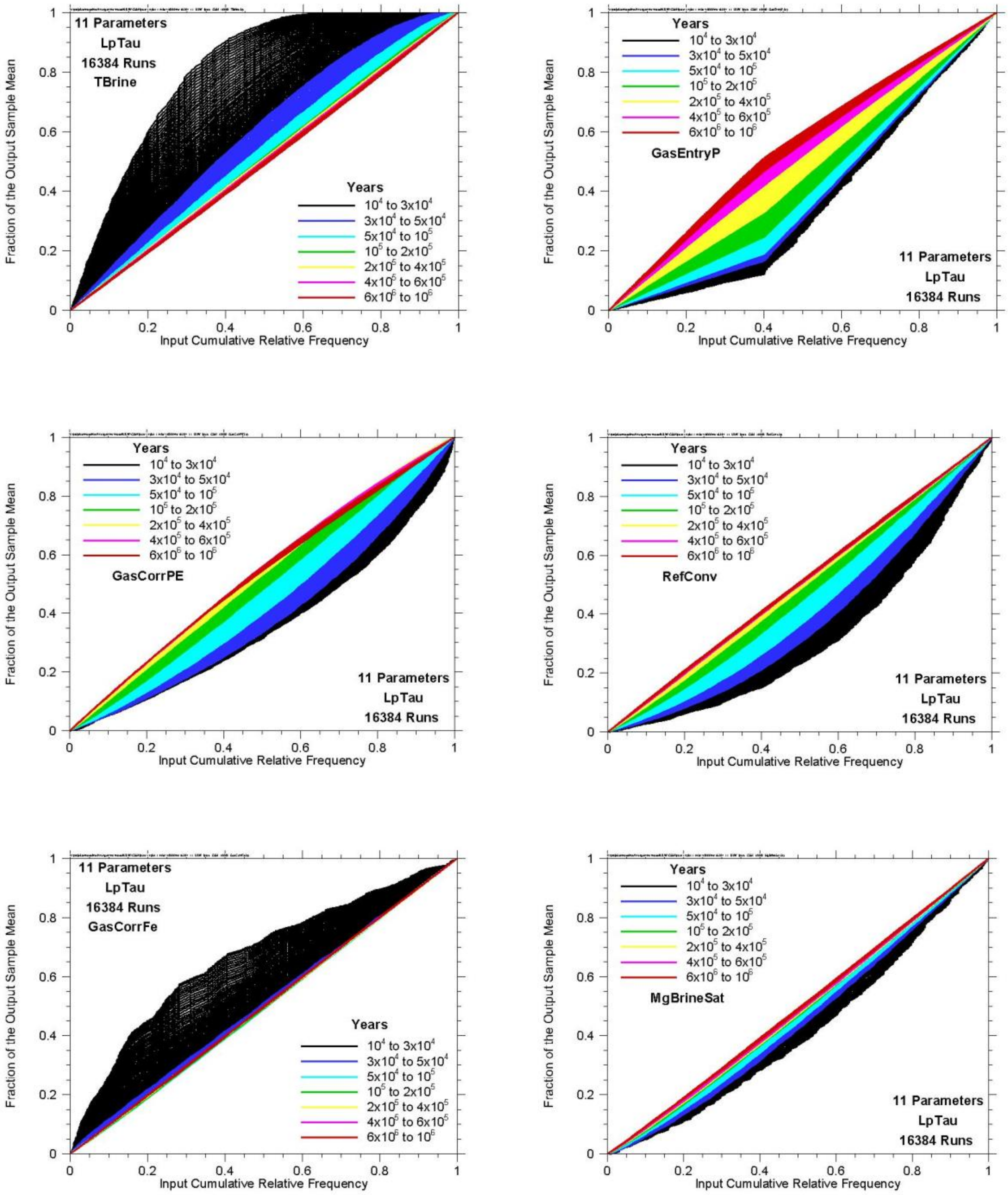
The time-dependent CSM plots attained from the parameters GasCorrPE and RefConv show clearly expanded but narrower sets of curves, which suggests a reduced significance of these parameters. The parameters BrineMgSat, RGConv and AEBGasProd have rather narrow sets of curves close to the diagonal, indicating a low relevance of these parameters. NABGasProd seems to have no importance as the CSM curves attained from this parameter show nearly no deviation from the diagonal. The same applies to GasCorrFe if the black curves for very early times are disregarded.

The sets of curves for all parameters except AEBConv, GasEntryP and CasCorrPE expand over only one side of the diagonal, which means that they have unique monotonic influence on the model. This influence is positive for all parameters except TBrine and GasCorrFe.

Figure 3 shows that Quasi-Random LpTau sampling produces more robust CSM plots than random sampling. The figure depicts the CSM plots of LpTau and random sets for all 11 parameters using 2048 and 4096 runs at 10^5 years. The CSM plots obtained using random sampling show that the deviations between the different sets with the same number of runs are bigger compared to the ones using LpTau sampling. For the set with LpTau sampling, a good convergence can be reached with about 2000 runs as the curves produced from the sets with 2000 and 4000 runs for most parameters closely agree. Figure 4 shows that a similar agreement of the CSM curves using random sampling is only achieved with two to four times higher sample sizes.

Figure 2: Time-Dependent CSM Analysis for Each Parameter





11 Parameters
LpTau
16384 Runs
TBrine
GasEntryP
GasCorrPE
RefConv
GasCorrFe
MgBrineSat
Years
10^4 to $3x10^4$
$3x10^4$ to $5x10^4$
$5x10^4$ to 10^5
10^5 to $2x10^5$
$2x10^5$ to $4x10^5$
$4x10^5$ to $6x10^5$
$6x10^6$ to 10^6
Fraction of the Output Sample Mean
Input Cumulative Relative Frequency

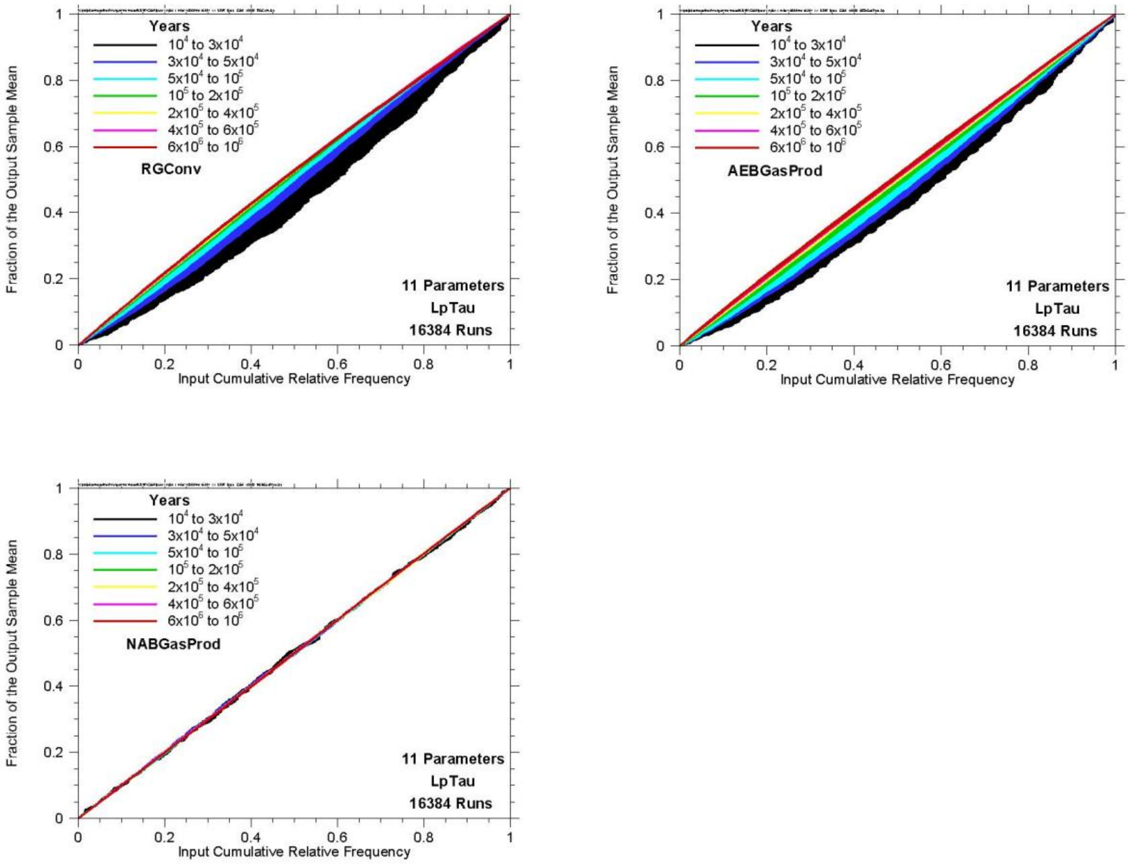


Figure 3: CSM Plots of the LpTau and Random Sets using 2048 and 4096 Runs at 10^5 Years

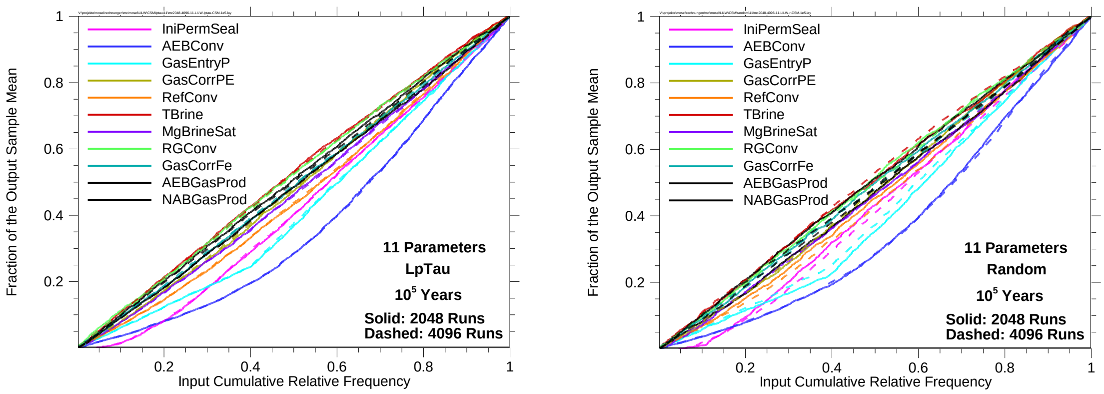
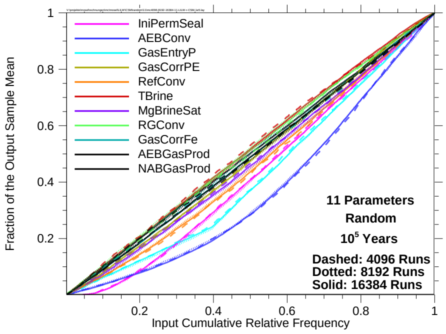


Figure 4: CSM Plots of the Random Set using 4096, 8192 and 16384 Runs at 10^5 Years



6.2. SRRC

Figure 5 shows the time-dependent SRRC coefficient values for all 11 parameters with LpTau and random sampling using 2048 and 4096 runs. The findings obtained with the SRRC method are similar to those derived from the CSM plots. The parameters IniPermSeal, AEBConv and TBrine and GasEntryP, which produce the most outstanding CSM plots, also have the most conspicuous SRRC curves and reach the highest absolute maxima. Like the CSM plot, the SRRC values obtained for TBrine indicate the highest importance in the early phase. The importance of IniPermSeal decreases with time, but the parameter still plays a role at the end of the simulation. The SRRC curves of GasCorrPE, RefConv, BrineMgSat and RGConv have less pronounced shapes. GasCorrFe, AEBGasProd and NABGasProd seem to have little importance as their SRRC coefficient values are close to zero.

The SRRC curves of AEBConv, GasEntryP, GasCorrPE, RefConv and TBrine cross the zero line, which means that, according to the SRRC evaluation, these parameters change their direction of influence at some point in time. Only AEBConv, GasEntryP and GasCorrPE, however, reach significant values on the opposite side. This is in line with the findings from the CSM plots.

As with the CSM analysis, the deviations of the SRRC coefficients between the different sets with the same number of runs are bigger using random sampling compared to the ones utilizing LpTau sampling (see Figure 5). For random sampling, there are still bigger deviations between the sets with about 8000 and 16000 runs compared to LpTau sampling using about 2000 and 4000 runs (compare Figure 5 and Figure 6). Figure 6 shows the SRRC curves using random sampling and about 4000, 8000 and 16000 simulations.

Figure 5: Time-dependent SRRC Ranking Coefficients of the LpTau and Random Sets using 2048 and 4096 Runs

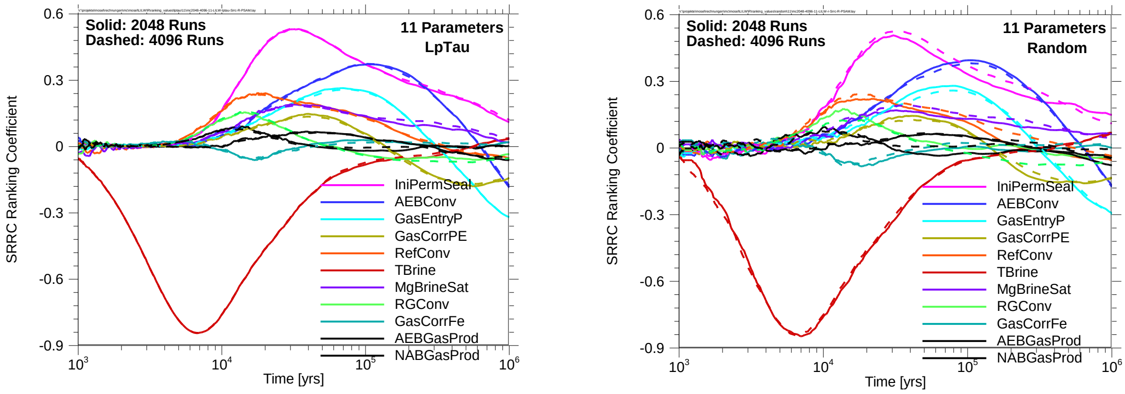
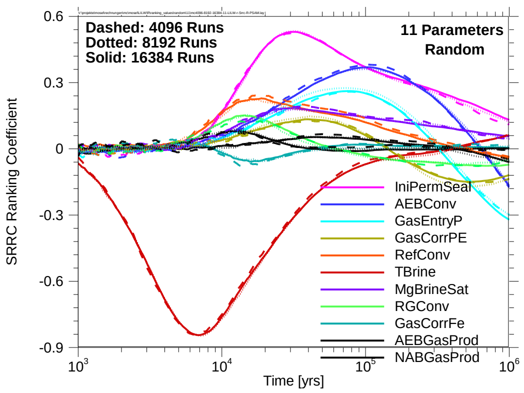


Figure 6: Time-dependent SRRC Ranking Coefficients of the Random Set using 4096, 8192 and 16384 Runs



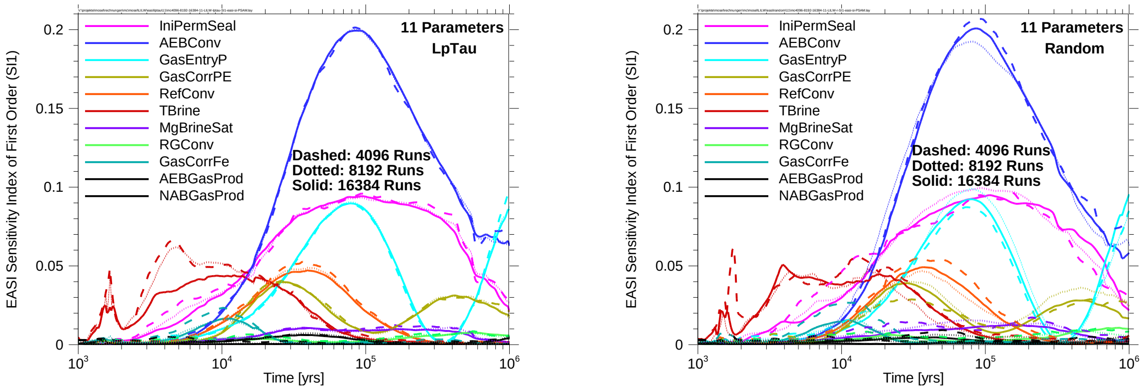
6.3. EASI

In Figure 7, the time curves of SI1 obtained with EASI for all 11 parameters are shown. The parameter AEBConv dominates the figure from about $2 \cdot 10^4$ years until the end of the scenario. The maximum SI1 values of IniPermSeal and GasEntryP are about half as high as that of AEBConv. The SI1 of TBrine is even lower in maximum, though dominating in the early phase. These results are different from those obtained with the CSM and SRRC analysis, which identified IniPermSeal and TBrine as more important than AEBConv, at least for the first 50 000 years of the simulation period.

The SI1's of RefConv and GasCorrPE go up to 0.05 and 0.04, respectively, which can be interpreted as a reduced importance of these parameters. The SI1 of GasCorrFe goes a little above 0.015 at the beginning of the simulation, which can be taken as some little significance. The SI1's of the rest of the parameters (BrineMgSat, AEBGasProd and NABGasProd) remain below 0.01, which seems to indicate that these parameters are insignificant.

As with the CSM and SRRC analysis, the deviations of the EASI SI1 indices between the different sets using random sampling are bigger compared to the ones obtained using LpTau sampling. Figure 7 also shows the results for the sets using random sampling and same number of runs as for LpTau sampling in this figure. It seems that with about 8000 runs, good convergence and smoothness of the SI1 indices can be achieved using LpTau sampling.

Figure 7: Time-dependent EASI SI1 of the LpTau and Random Sets using 4096, 8192 and 16384 Runs



7. SUMMARY AND CONCLUSIONS

In this paper, we investigated the performance of three different types of methods for calculation of sensitivity measures in combination with different sampling schemes on the basis of a PA model for low- and intermediate-level radioactive waste in rock salt. This PA model behaves nearly non-continuously or quasi-discretely as a result of the dissolution and nearly sudden failure of the seal in the near field. When this barrier fails, a sudden high release of radionuclides, i.e., a jump in the model output occurs. The investigated sensitivity analysis methods include a graphical method (CSM plot), a regression-based (SRRC) method and a variance-based method (EASI). With these different methods, a time-dependent analysis was performed, in which the annual dose values for a number of discrete time points, distributed over a time interval of 10^6 years, were analyzed. In addition, results obtained using LpTau sampling were compared to the ones using random sampling. Samples of different sizes with 11 parameters were examined.

For random sampling, the differences between the sensitivity measures obtained with different numbers of runs are bigger compared to those calculated using LpTau sampling. This means that the LpTau-based investigations show satisfying convergence at smaller sample sizes than random-based investigations. For the model under consideration, this confirms the assumption that quasi-random sequences are advantageous for sensitivity analysis. For CSM and SRRC analysis and with LpTau sampling, a sample size of about 2000 for the considered PA model with 11 parameters seems to be sufficient for good convergence of the sensitivity measures. For the EASI method, it appears that the sample size should be about 8000 to obtain comparably smooth curves and good convergence.

The results obtained with CSM and SRRC analysis are fairly comparable. Both methods identify the same parameters as important. While CSM plots give an optical visualization of the sensitivity, the SRRC provide a quantitative measure, although it should be kept in mind that the rank transformation destroys some quantitative information.

The EASI results, however, differ from those obtained with CSM and SRRC. They assign the dominating role to a parameter that seemed to be of secondary importance in the other evaluations. Specifically in the early phase below 10^4 years, the EASI results seem to be of low robustness, and therefore, higher confidence might be given to the SRRC calculations. In this phase, the release of radionuclides is just starting and only a few simulations lead to a non-zero release at all.

The differences between the evaluations with EASI and with SRRC/CSM may be due to the fact that changes in the model output are squared in the computation of variance-based sensitivity measures and that only a few output values may dominate the computed sensitivity indices. In a different investigation we demonstrate that the EASI results get more similar to those obtained with SRRC and more robust in the early phase if an output transformation is applied [6]. However, despite of the transformation, one parameter that obviously has some influence on the model sensitivities was not identified as important by any of the methods under investigation. This parameter is one of those parameters that control the quasi-discrete behavior of the PA model.

From each type of evaluation valuable information could be obtained in terms of parameter ranking and understanding of the system behavior. Consequently, it can be inferred that for the investigated PA model with strong nonlinear system behavior, it is very important to explore the parameter space as homogeneously as possible to obtain robust sensitivity measures. In addition, it is very helpful to perform sensitivity analysis of the model with different types of methods.

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