Deliverable 10.4: Methodological Approaches to Uncertainty and Sensitivity Analysis

Work Package 10: Strategic Study WP – Uncertainty Management Multi-Actor Network (UMAN)

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Executive Summary

The UMAN work package within EURAD is dedicated to the management of uncertainties potentially relevant to the safety of different radioactive waste management stages and programmes. UMAN is focussed on developing a common understanding among European Waste Management Organisations (WMOs), Technical Safety Organisations (TSOs) and Research Entities (REs) and civil society of strategies and approaches for managing uncertainties by sharing knowledge and identifying remaining and emerging issues. The overall goal defined for its Task 2 “Strategies, Approaches and Tools” is to compile, review, compare and refine strategies, approaches and tools for the management of uncertainties in the safety analysis and the safety case that are being used, planned to be used or being developed in different countries. The goal of Subtask 2.3 is to investigate how typical numerical performance assessment (PA) models can best be analysed in view of uncertainty and sensitivity with classical and modern methods and, where sensible, to coordinate, initiate or recommend the development of appropriate computational tools:

- identification of methods for uncertainty and sensitivity analysis already applied in repository PA
- analysis of the general understanding of these methods and their outcome
- identification of specific strengths and weaknesses of these methods
- suggestions for application of newly developed methods
- suggestions for refinement of methods

This report presents the findings of the EC UMAN project regarding to methodological approaches used in the uncertainty and sensitivity analysis. The work also includes examples of the application of different methods to existing sets of probabilistic PA calculations. The major input to this report comes from a dedicated UMAN questionnaire.

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Glossary

This section defines some common terms used in this document, with a focus on uncertainties.

Numerical Simulator: The implementation of a (deterministic) function, called the model, in computer code that maps input parameters to the simulation results.

Sample: The realization of multiple independent copies of a random variable/vector. A single realization is also called run or observation.

Monte Carlo Simulation: The process of sampling from the input distribution and promoting each run through the numerical simulator to obtain an empirical distribution of the output; the universal approach to Forward UQ

Quantity-Of-Interest: A scalar parameter, derived from the model output, which is used for uncertainty / sensitivity considerations. It needs to be specified if the simulator returns, e.g., time-series.

Uncertainty Quantification: The investigation of different sources and levels of uncertainty in numerical simulations.

Forward Uncertainty Quantification: The process of quantifying the uncertainties in quantities-of-interest by propagating the uncertainties in input parameters through the numerical simulation model.

I**nverse Uncertainty Quantification**: The process of inversely quantifying input uncertainties based on experimental data in order improve ad-hoc specifications of the input uncertainty information.

Uncertainty Analysis: The process of exploring the uncertainty in the model output/quantity-of-interest.

Sensitivity Analysis: The process of assessing the dependency of the model output/quantity-of-interest on the model input, and of investigating how important each model input is in determining the output.

Screening: The process of identifying non-essential model input parameters, hence reducing the input dimension.

Uncertainty: Lack of objective information (evidence) or subjective information (knowledge)

Aleatory Uncertainty: The stochastic part of the uncertainty of an input parameter that forms an intrinsic property of the parameter and that cannot be reduced. An aleatory random variable represents the possible outcome of an observation of the quantity.

Epistemic Uncertainty: The part of the uncertainty of an input parameter resulting from limited knowledge of the natural conditions and processes that can in principle be reduced by obtaining more information. An epistemic random variable represents the state of knowledge about the quantity.

Input Uncertainty: A mathematical description of the uncertainty in the input parameters. This may include parameter ranges, mean values and variances, the specification of marginal distributions and joint distributions. Depending on the context, inputs may also be called parameters, features or factors.

Output Uncertainty: The result of propagating the input uncertainty through the model. If one interprets the input parameters as random quantities, the simulation output becomes a random quantity as well.

Verification: The process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model.

Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

Qualification: The process of determining the degree to which results of the numerical simulator are in line with the phenomenological basis, a weaker form of validation which takes the spatiotemporal limitations of experiments into account.

1. Introduction

The work package (WP) UMAN within EURAD is dedicated to the management of uncertainties potentially relevant to the safety of different radioactive waste management (RWM) stages and programmes. This WP allowed identifying the contribution of past and on-going RD&D projects to the overall management of uncertainties as well as remaining and emerging issues associated with uncertainty management that, e.g., could be addressed in subsequent waves of EURAD. Actors taken into account comprise of waste management organizations (WMO), technical support organizations (TSO), research entities (RE) and the Civil Society. Major UMAN goals as defined in the project proposal are:

- "Develop a common understanding among the different categories of actors on uncertainty management and how it relates to risk & safety. In cases where a common understanding is beyond reach, the objective is to achieve mutual understanding on why views on uncertainties and their management are different for different actors.
- Share knowledge/know-how and discuss common methodological/strategical challenging issues on uncertainty management.
- Identify the contribution of past & on-going RD&D projects to the overall management of uncertainties.
- Identify remaining and emerging issues and needs associated with uncertainty management."

Another citation from the UMAN project proposal nicely summarizes the role of uncertainties, i.e. why the WP has been initiated: "Decisions associated with radioactive waste management programmes are made in the presence of irreducible and reducible uncertainties. Several choices made based on limited information in early programme phases may also have to be confirmed before or during the construction and operation of the facility. At the end of the process, uncertainties will inevitably remain but it should be demonstrated that these uncertainties do not undermine safety arguments. Hence, the management of uncertainties is a key issue when developing and reviewing the safety case of waste management facilities and, in particular, of waste disposal facilities due to the long timescales during which the radiotoxicity of the waste remains significant."

The overall goal defined for Task 2 "Strategies, Approaches and Tools" within UMAN is to compile, review, compare and refine strategies, approaches and tools for the management of uncertainties in the safety analysis and the safety case that are being used, planned to be used or being developed in different countries.

1.1 Objective and subjects of this report

The goal of the work reported in this deliverable is to investigate how typical numerical PA models can best be analysed in view of uncertainty and sensitivity with classical and modern methods and, where sensible, to coordinate, initiate or recommend the development of appropriate computational tools:

- identification of methods for uncertainty and sensitivity analysis already applied in repository PA
- analysis of the general understanding of these methods and their outcome
- identification of specific strengths and weaknesses of these methods
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2. Modelling methodology

Let us first review the questions what a model is, and especially, what is meant by simulation. Wharton (2022) lists the following two items as informal definition:

- models have referents,

- a model differs from its referent.

What the model refers to might be another model. If a model and its referent are the same then we should speak of a copy or a clone, but not a model (The idea of a digital twin, behaving exactly like the physical system, is still a model as the realms (physical and digital) are different). There is always the danger of mixing models and facts in scientific discussion and communication with stakeholders.

Rosen (1991) and Louie (2009) draw the following picture on modelling methodology: a natural system offers cause-and-effect relations while a formal system offers theoretical inferences. There are encoding and decoding operations to connect the systems, especially the pathway of the concatenated operations encode-infer-decode offers a way to simulate: the natural causes and effects can be inferred from the formal system; while the concatenation decode-cause-encode is a way to verify that the conclusions from the formal system are found in nature. If one translates "encoding" with observing physical quantities, and "decoding" with controlling physical states, these maps are far from being one-to-one: There are uncontrollable and/or unobservable states in the natural system. Hence, the formal system, while it refers to the natural system via the encoding/decoding operations, is not an exact copy of the natural system.

2.1 Simulation

A simulation model is always located within the realm of formal inference. Only then, Wigner's "unreasonable effectiveness of mathematics" can come into effect, as mathematics is main language for performing formal inference.

For a simulation model, the following layers of abstraction from the physical system to the computational implementation can be identified,

1. Conceptual model (which parts of the natural system should be considered?),
2. Physico-chemical description of the processes involved,
3. Mathematical model (e.g., in form of differential equations),
4. Numerical model (algebraic equations, approximate solution algorithms),
5. Machine code (computer software).

Each modelling layer provides a description of the relevant events and processes, with varying degree of abstraction. In each layer, errors or wrong decision are possible and probable. Hence, a quality assurance with a management of mistakes needs to be implemented when dealing with simulation models.

Oberkampf & Roy (2010) comment on the layers of abstraction:

The conceptual model specifies the physical system, the system surroundings, and the phenomena of interest; the operating environment of the system and its domain of intended use; the physical assumptions that simplify the system and the phenomena of interest; the system response quantities of interest; and the accuracy requirements for the response quantities of interest.

The mathematical model is derived from the conceptual model: it is a set of mathematical and logical relations that represent the physical system of interest and its responses to the environment and the initial conditions of the system. A system of partial differential equations (PDEs), integral equations, boundary conditions and initial conditions, material properties, and excitation equations usually describes the mathematical model.

The computational model can be obtained from the numerical implementation of the mathematical model, a process that may result in a set of discretized equations and solution algorithms, and then these equations and algorithms are programmed into a computer. Another way to describe the computational model is that it is a mapping of the mathematical model into a software package that, when combined with the proper input, produces simulation results.

Simulation models are not restricted to be solutions of differential equations. There are alternative approaches to simulation models (see also Morris (2012)):

- time-dependent processes may be modelled by ordinary differential equations, defined in terms of derivatives with respect to time only,
- spatio-temporal processes may be modelled by partial differential equations that also include derivatives with respect to other quantities, like spatial dimensions,
- agent-based models that explicitly represent the actions and interactions of autonomous units in a network, e.g., of vehicular traffic,
- discrete event simulations based on a chronological sequence of events, e.g., for queuing systems,
- large nonlinear systems, e.g., equations of state that describe a thermodynamic equilibrium point under a given set of physical conditions.

One may also distinguish between deterministic models in which all quantities can be expressed with complete certainty, and stochastic models where unpredictable random quantities form an intrinsic part of the model, e.g., a discrete event simulator will include a random arrival process.

The use of stochastic models in a Monte Carlo simulation context poses further challenges: One may process the output directly, and then one must take into account the presence of latent variables. Alternatively, one calls the stochastic model repeatedly with the same parameter set, and then uses the average value as output of the simulator, or one treats the whole sample as empirical distribution and feeds it into the ensuing analysis as a functional argument.

Triebel (1989) offers the following informal criteria for mathematical models, which also are of interest for simulation models:

1. A model is good if it works. As such, there is no right or wrong in modelling, just useable or unsuitable models. Here “useable” is used in the sense that physical effects in question can be described sufficiently well by the model.
2. A model should be as simple as possible. There should be no reason to replace a working model with a more complex one, unless one finds good physical evidence to do so.
3. There exists a hierarchy of physical theories and associated mathematical models with respect to the part of reality being described, and the precision being offered by the model. Hence models yield only approximate descriptions.
4. Models may be able to forecast and predict new effects.

Different mathematical approaches require different strategies to end up with a software implementation. A numerical solution might only provide an approximation of the theoretical results.

2.2 Uncertainty Management and Safety Strategy

When making decisions in the presence of uncertainties, these uncertainties need to be carefully identified and tracked. It is recommended that a register of significant uncertainties is required as part of the safety analysis for a disposal system. Once uncertainties have been identified, the question of their further management arises. It is thus also recommended that the developer of the disposal facility should present a clear forward strategy for managing uncertainties. A further type of uncertainty can be identified when presenting and communicating results (linguistic uncertainty). Here suitable guidance may help in reducing misunderstandings (e.g., Mastrandrea et al. (2010)).

Developing such an uncertainty management strategy involves asking at least the following questions for each uncertainty:

- Is the uncertainty important?
- Can the uncertainty be avoided, mitigated, or reduced?
- Can the uncertainty be quantified?

The distinction between aleatory or epistemic uncertainty depends on the (sometimes subjective) setting of system limits, boundary conditions, etc. Hence, the following classification might be more relevant for safety and performance assessments, by attributing the uncertainty to the following classes:

- Modelling uncertainties,
- Scenario uncertainties,

- Parameter/data uncertainties.

If one deals with a finite set of modelling or scenario uncertainties these can be mapped into discrete parameters, so that all uncertainty presents itself as parametric. For parameter uncertainties, there are quantitative methods available. The typical question of how uncertain the results are can be answered by the methods of uncertainty analysis; the question of which input parameters are especially dominant or important for the uncertainty of the result by sensitivity analysis.

Hofer (2018) addresses the search for potentially important epistemic uncertainties as a first step in performing uncertainty management for decision-making models. This should be implemented by inspecting all stages on the path from the assessment question to the computer model result:

When defining a scenario, simplifications and omissions in the scenario description and their potential impact on modelling results should be documented and assessed. It is clear that numerical values used in calculations are subject to errors of reporting, detection, measurement and interpretation. If an inflexible model is employed, it might not cope with input values from alternative scenarios. For a conceptual model, intentional omissions and simplifications need to be scrutinized.

For the mathematical model, one must ask if the model equations represent the governing laws in a way that permits an adequate account of the effect of phenomena and mechanisms important for the model result. Moreover, one must check if the influence of the disturbances on the evolution of variables is sufficiently accounted for.

In the numerical model, accuracy and efficiency of approximate solutions may be controlled by error tolerances, discretization granularities (step / grid sizes) or regularization parameters. The influence of these hyper-parameter settings on the outcome is also of interest for assessing uncertainty.

A way to cope with uncertainties in the scenario and conceptual phases is to ask for the gap between what is known and what need to be known. A structural approach is developed in Ben-Haim (2006), based on the theory of information value; an expert-judgement-based approach is found in Hubbard (2014). Deliverable D10.3 (Brendler & Pospiech 2020) suggests fishbone diagrams to structure the impact of uncertainties, among other methods.

The NUSAP (Numeral, Unit, Spread, Assessment and Pedigree) methodology for assessing the quality of the uncertainty assumptions considers different dimensions (van der Sluijs 2017). Special attention is given here to the pedigree of the underlying knowledge. One quantifies if the information comes from an established theory; if the numerical value (and its spread) is accepted by the peers; if the data are obtained from measurements, historical records, or guessing; if competing schools have different views on the information.

Hicks et al. (2020) present uncertainty management strategies with special attention to disposal projects referencing the earlier work of Vigfusson et al. (2007). There, the options of reducing uncertainties e.g. by research, avoiding it or mitigating its effects by siting or design measures are mentioned. With a focus on radioactive disposal, Kreusch et al. (2019) list the following strategies for managing uncertainties: a) increasing the visibility of uncertainties as part of a good risk governance; b) avoiding uncertainties by recurring to established technical solutions; c) mitigating uncertainties by further research activities; and d) strengthening the ability to cope with uncertainties via robustness and resilience concepts. One observes that both societal as well as technical approaches are part of this management strategy. In any case, a prerequisite to “managing” an uncertainty is evaluating its magnitude and impact, e.g., in safety assessments. Eckhardt (2021) suggests a scheme informing decisions on uncertainty management based on the categories “safety relevance”, “magnitude”, “quality of statements” and “potential to address the uncertainty”.

3. Uncertainty Analysis

Wu et al. (2018) offer an overview of terms used in simulation modelling and computer experiments, see *Figure 1*. Uncertainty analysis can be described in terms of forward and inverse uncertainty quantification (UQ). While the forward UQ produces predictions of the results as a random quantity, the inverse or backward UQ tries to reduce the input uncertainty with the help of predictions and experiments. Hence, sensitivity analysis can be seen as part of this backward process.

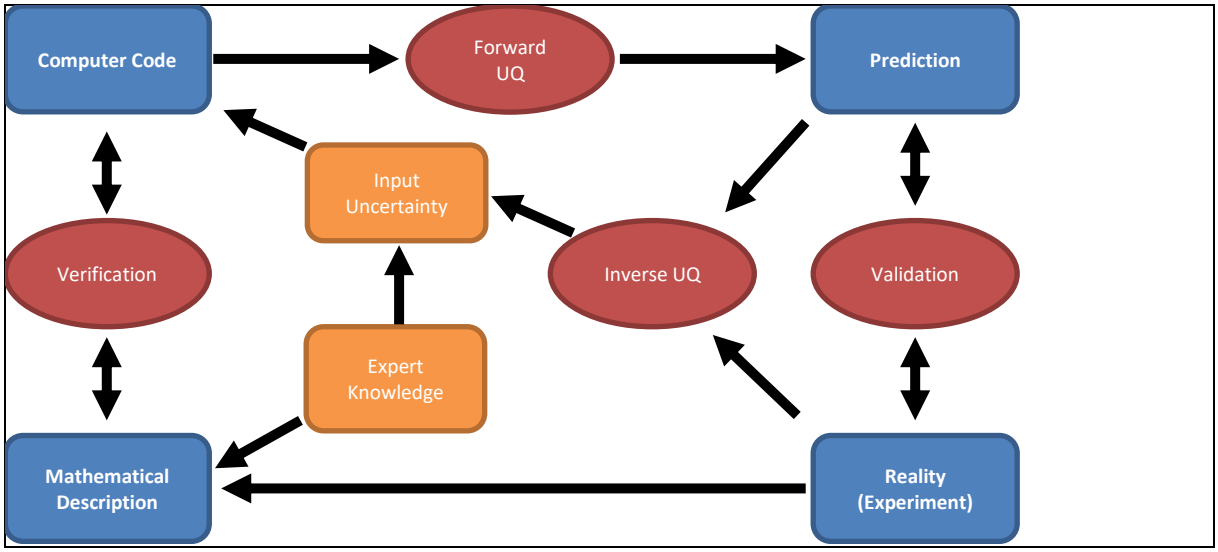

Figure 1 – Terms in Modelling, Simulation and Computer Experiments (after Wu et al. (2018)*).*

In order to perform an uncertainty analysis, Hofer (2018) breaks down the analysis in the following steps. As a first step, one needs to quantify the uncertainty, both in the input data and in the numerical model. Then, one propagates the uncertainty though the numerical model, which typically involves Monte Carlo sampling. This step assumes that the uncertainty quantification yields a probabilistic description of the input and model uncertainties. Having available an input/output sample, the third step consists of estimating the output uncertainty using a graphical display of the modelling results. The last two steps then involve the ranking of uncertainties and the sensitivity analysis.

Input uncertainties can be described using an increasing level of complexity, depending on the present state of knowledge,

- nominal/reference point, most probable value
- intervals, ranges between minimal and maximal values
- correlations and interdependencies
- fully specified probability distributions, marginal and joint distributions
- p-boxes (Ferson et al. 2003), covering a whole range of distributions (imprecise probabilities)
- fuzzy logic (Zadeh 1964), using necessity and possibility functions which are linked via a complement operation
- Dempster-Shafer evidence theory (Shafer 1976), specifying the probability that the truth is contained in a (so-called focal) set; using belief and plausibility functions

Some of these more complex descriptions of uncertainty are discussed in Augustin et al. (2014). For many of these descriptions of uncertainty, a maximum entropy principle or a defuzzification step is available to obtain a sample for a Monte Carlo simulation. However, care should be taken in this step: Suppose that one only specifies a parameter range with minimum and maximum values. Soize (2017) warns that putting uniform distributions either on a resistance or on its reciprocal quantity, a conductance, will have major impact on any output distribution derived from these parameters, although the extremal limits are the same.

3.1 Uncertainty Propagation

De Rocquigny (2012) calls Monte-Carlo simulations the universal approach for approximate numerical integration or empirical output distributions. Monte-Carlo methods can be modified by using variance reduction techniques like quasi-Monte-Carlo sampling with low discrepancy series, or importance sampling, which might be iterated to obtain Multi-Level Monte-Carlo methods. Alternatives are available using Taylor approximation (law of uncertainty propagation), numerical integration (quadrature rules for computing expectations), or structural reliability methods like first-/second-order reliability methods (FORM/SORM) identifying the most probable point of failure (Der Kiureghian 2004).

In order to put Monte-Carlo methods in uncertainty analysis and global sensitivity analysis to work, the following assumptions have to be met:

1. uncertainties can be described by probability distribution functions

2. the generated input parameter sample $(x_i^1, x_i^2, \ldots, x_i^d), i = 1, \ldots, n$ approximates the input distribution $\mathbb{P}_X$ well enough. Here d denotes the number of inputs, n is the sample size and i runs through all realisations.

3. the computational model yields the output sample $(y_i) = g(x_i^1, x_i^2, \ldots, x_i^d), i = 1, \ldots, n$ that approximates the output distribution $\mathbb{P}_Y$ well enough.

Therefore, the forward path of uncertainty quantification consists in most cases of the following steps:

- Identification of uncertain input parameters
- Identification of probabilistic distribution functions, dependences, correlations
- Sampling: Monte-Carlo-Generation of equally probabilistic parameter sets
- Model calculations for each parameter set yields a set of output results
- Output statistics: uncertainty analysis

The backward path of uncertainty quantification, which takes the observed output distribution to infer input distributions is called inverse UQ. It consists of methods like parameter estimation and model calibration. Statistics for the relationship between input and output are offered by the tools of sensitivity analysis.

3.2 Characterizing Uncertainties

Given a Monte Carlo sample, one can derive the following quantities (Bolado & Badea 2006)

- Empirical cumulative distribution/survival functions, quantiles, densities (via histogram or kernel density smoothing);
- Central tendencies: mean (arithmetic, geometric, harmonic), median, mode;
- Dispersion measures: range, interquartile range, variance, standard deviation;
- Shape measures: skewness, kurtosis.

For graphical representation, box plots (and its variants, violin plots etc.) can compactly represent probabilities, while for a graphical comparison of a distribution with a member of a parameterized family of distributions probability/probability (PP) or quantile/quantile (QQ) plots are available.

Dealing with time series, one should communicate results on selected quantities of interest.

4. Sensitivity Analysis Methods

To demonstrate techniques, the PSACOIN Level E example is considered in this report. In various publications (see Saltelli & Tarantola (2002) for a review), this code (OECD NEA 1989) is used both for benchmarking Monte Carlo simulations and for sensitivity analysis methods. It simulates the radiological dose to humans over geological time scales due to the underground migration of radionuclides from a hypothetical nuclear waste disposal site through a system of idealised natural and engineered barriers. The model has a total of thirty-three parameters, twelve of which are taken as independent uncertain

parameters. The parameter uncertainties are uniformly or log-uniformly distributed. The input parameters split into four groups, three parameter modelling the contaminant source, two geosphere layers with four parameters each and a biosphere parameter. *Table 1* lists the uncertain parameters and their ranges.

Table 1 – Level E: Uncertain parameters and their ranges.

Parameter		Description	Distribution	Range	Unit
1	T	Containment time (source)	Uniform	10^2…10^3	a
2	k_I	Leach rate for Iodine (source)	Log-Uniform	10^{-3}…10^{-2}	1/a
3	k_C	Leach rate for Np decay chain (source)	Log-Uniform	10^{-6}…10^{-5}	1/a
4	v^1	Water velocity (1st layer)	Log-Uniform	10^{-3}…10^{-1}	m/a
5	l^1	Length (1st layer)	Uniform	100…500	m
6	R_I^1	Iodine retardation (1st layer)	Uniform	1…5	-
7	γ_C^1	Np chain retardation multiplier (1st layer)	Uniform	3…30	.
8	v^2	Water velocity (2nd layer)	Log-Uniform	10^{-2}…10^{-1}	m/a
9	l^2	Length (2nd layer)	Uniform	50…200	m
10	R_I^2	Iodine retardation (2nd layer)	Uniform	1…5	-
11	γ_C^2	Np chain retardation multiplier (2nd layer)	Uniform	3…30	-
12	W	Stream flow rate (biosphere)	Log-Uniform	10^5…10^7	m^3/a

4.1 Local Sensitivity Methods

The behaviour of a simulator model is studied around a default or reference value / base case / working point. For this, partial derivatives or difference quotients varying one input parameter at a time (OAT) are considered.

One obtains a linear approximation of the local output response surface. The main problem with this approach is that parameters have different units and might not be comparable. A suggestion to deal with this problem is the differential importance measure (DIM) of Borgonovo & Apostolakis (2001),

$$DIM_i = \frac{\partial g(x^0)}{\partial x_i} dx_i \left(\sum_{i=1}^{d} \frac{\partial g(x^0)}{\partial x_j} dx_j \right)^{-1}$$

If automatic/algorithmic differentiation methods are available or the output is already the solution of a system of differential equations, then measures based on partial derivatives become attractive. Here local sensitivities of input parameters might be obtained from adjoint methods (Cacuci 1981). Another way to take local derivatives is to switch to complex arithmetics where derivatives of analytical functions can be easily found in the complex part (Lyness & Moler 1967).

4.2 Screening

The purpose of a screening method is to identify uninfluential input parameters with relative few model evaluations. The costs are in most cases linear in the input dimension. These methods require parameter ranges to be specified.

4.2.1 Tornado diagrams

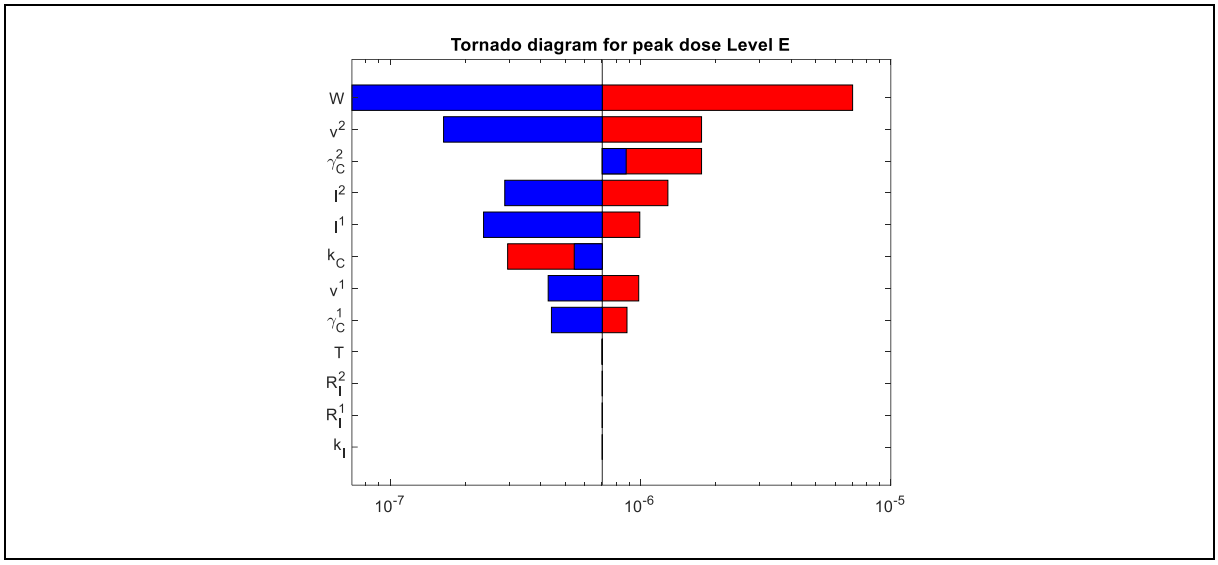

Figure 2 – Tornado diagram: Deviations from the base case, blue codes favourable, red risky input settings. Some inputs exhibit non-monotonic behaviour.

This type of diagram is discussed in Eschenbach (1992). It requires the definition of a base case, together with minimum/favourable and maximum/unfavourable values. Global one-factor at-a-time (OAT) variations from the base case to the extremes are computed. The deviations in the output are sorted and presented in a horizontal bar plot so that the parameter which induces the largest change in the output compared with the base case is presented first. One can color-code the two directions (towards the favourable or unfavourable value, respectively) to obtain a direction of change. For the Level E example (OECD NEA 1989), in *Figure 2* one observes four parameters with no contribution, but also two where the behaviour is nonlinear (for k_C and γ_C^2 both arms of the swirl point in the same direction). In all other cases, modifying the input value to a favourable setting actually decreases the output value. Note that the output is presented on a log scale.

4.2.2 Morris Method

The Morris Method uses randomized OAT designs. The high dimensional input space is partitioned into small hypercubes. One randomly selects some of these hypercubes. In each of these selected hypercubes, OAT designs, like radial design or winding stairs design, are used along the vertices. The difference in the outputs between the base case and the alternative case per factor is then averaged. For a radial design, the base case is the same for all factors, while in a winding-stairs design the alternative case becomes the base case for the next factor. For capturing nonlinear and nonmonotonic trends, the absolute means $|\mu|$, the means of the absolute values μ^*, and the variances σ^2 of multiple OAT experiments are reported, see Campologo et al. (2007).

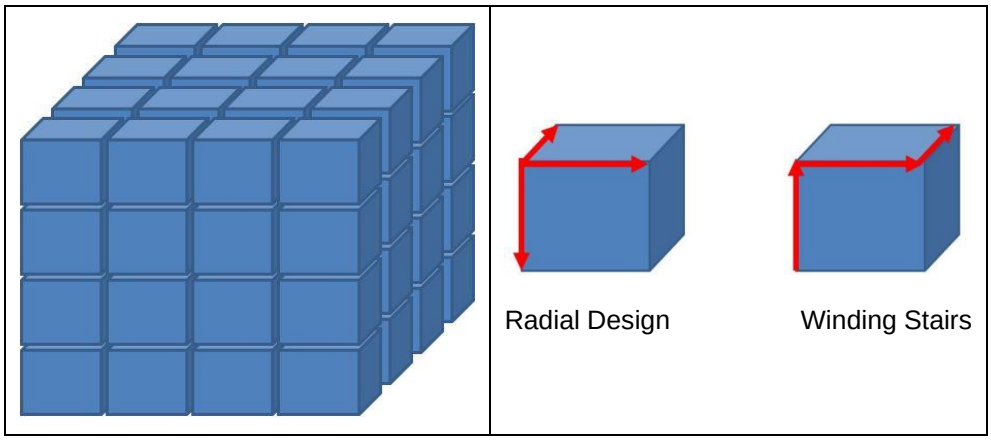

Figure 3 – Morris elementary effects. Hypercubes form a partition of the input space. On randomly selected ones, a radial or winding stairs design is computed.

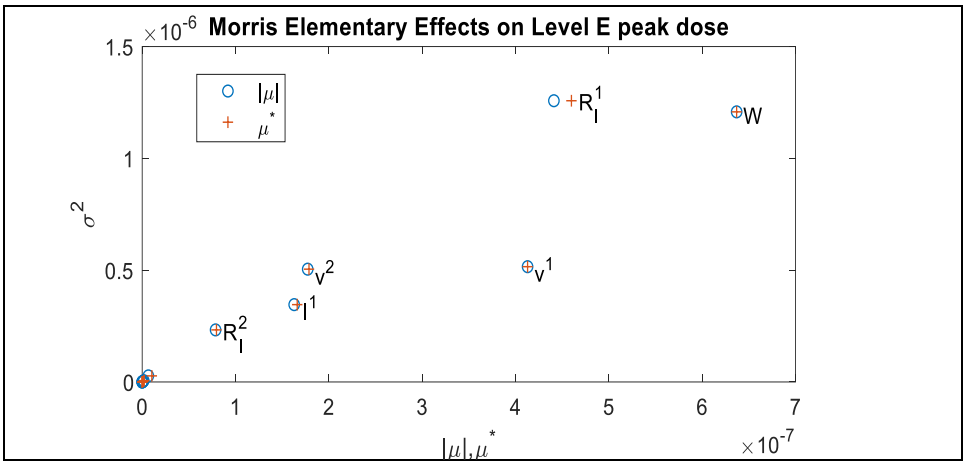

Figure 4 – Results for Morris elementary effects: Mean and variance of the (absolute) difference quotients are taken as sensitivity measures.

For the Level E example (OECD NEA 1989), by selecting 10 hypercubes out of 20 per dimension one can screen out six parameters (130 calls to the simulation model were required), see *Figure 4*. Note that R_I^1 shows up prominently (with a slight nonlinear effect, as $|\mu|$ and μ^* differ in this case), while the tornado diagram did not attribute any significance to this parameter. However, the values were reported using the average (and standard deviations) of 10 repetitions, using 20 intervals per dimension. This amounts to choosing 12*10 cubes out of possible 20^{12}, which provides a very bad coverage of the input parameter space. A remedy is to use variable distances between base and alternative points.

4.2.3 Sequential Bifurcation

For sequential bifurcation as introduced by Bettonvil & Kleijnen (1997), the inputs are partitioned into groups. Within each group, one assumes co-monotonic behaviour. One defines low and high values for each input parameter (ISO 1997 calls these “carefully estimated” extreme values). All the inputs for each group are cyclically changed from high to low and back (as demonstrated in *Figure 5* with three groups). Those outputs are then compared to outputs where the parameters not in the group remain the same: a large deviation in this finite change sensitivity index signals an important factor in the group. For closer inspection, the most interesting group with the largest absolute difference is refined by bifurcating the index into two subgroups which requires two more simulator calculations.

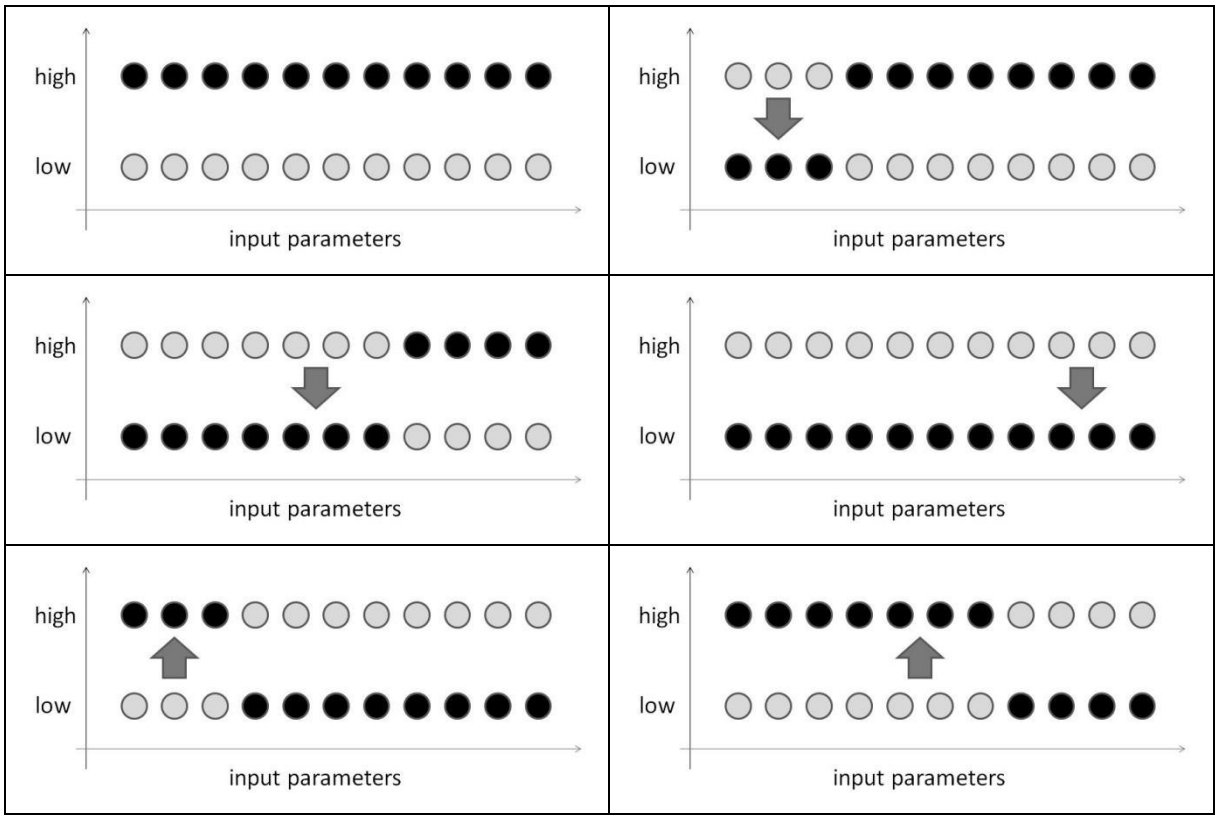

Figure 5 – Sequential bifurcation: The inputs are cyclically changed per group from a high water mark to a low water mark and back again.

Table 2 – Level E: Ranking from Sequential Bifurcation (Leftmost: important global change).

Original Scale	v^1	l^1	W	γ_C^1	R_I^1	l^2	R_I^2	v^2	k_I	T	k_C	γ_C^2
Log Output	W	v^1	l^1	R_I^1	γ_C^1	l^2	v^2	R_I^2	k_I	T	k_C	γ_C^2

Table 22 shows the ranking for sequential bifurcation with Level E, starting from four groups (containing each three parameters) until each group contains a single parameter. The ranking changes slightly when switching to a logarithmic scale. The last two highlighted parameters show a null effect.

4.2.4 Remarks and Outlook

The screening methods introduced above are model-driven: they require (a few) model evaluations. If the input dimension is large (say, d>200) then these approaches might not be attractive, and the data-driven tools of global sensitivity analysis (see next section) can offer a smaller computational budget that does not depend on the input dimension.

For sequential bifurcation, one may replace the finite change sensitivity indicator (from the grouped OAT design) with a variance-based indicator (using a pick-and-freeze design, see below).

Most screening methods are ad-hoc, with little theoretic underpinnings. The Morris method is linked to derivative-based sensitivity methods that in turn are connected to variance-based total effects.

Because of the informal character of the definition of these screening methods, if they are used to screen out certain model parameters which are then excluded from further uncertainty and sensitivity studies, this decision should be carefully assessed at later stages of the programme as part of an uncertainty management strategy. Moreover, note that these methods generally make implicit assumptions on the

model smoothness: Grid-based methods implicitly assume that off-grid points are behaving close to grid-points. Even deterministic models with bounding calculations need some monotonicity or convexity properties.

4.3 Global or Probabilistic Sensitivity Analysis

In contrast to the previous methods, it is assumed that a fully probabilistic description of the input uncertainty is available. Global methods study how the uncertainty is promoted through the simulation model, such that key drivers of uncertainty among the input parameters can be identified. To demonstrate data-driven techniques, a quasi-Monte Carlo sample of size 2^{13}=8192 for the Level E example is reanalysed, considering the outputs at all time-steps as quantities of interest.

4.3.1 Correlation analysis

The Pearson product moment correlation coefficient measures the strength and direction of a linear relationship between two variables. In technical terms, it compares the mean of the joint distribution with the product of the marginal means. Under input independence, it coincides with the standardized regression coefficient that is obtained from a least squares regression.

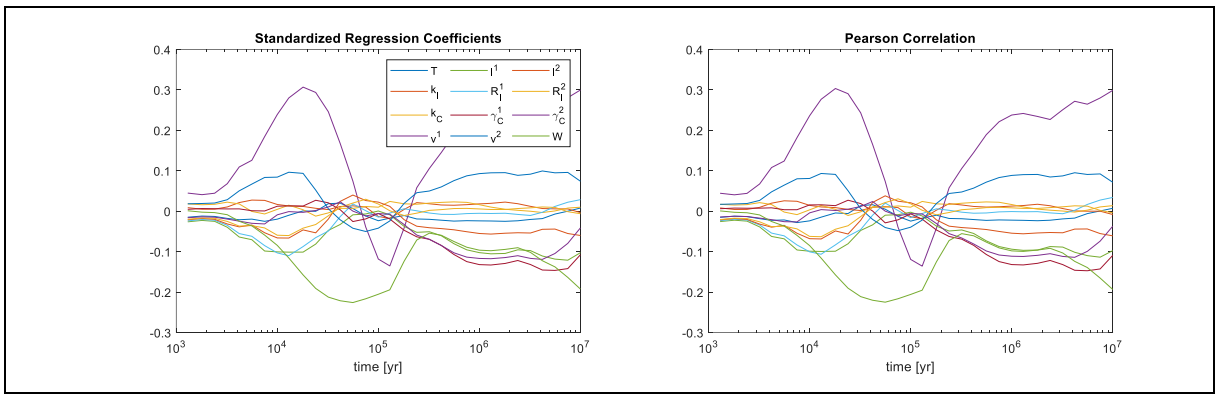

Figure 6 – Time dependent linear sensitivity: Left panel, standardized regression coefficients. Right panel, Pearson product moment correlation coefficients.

And indeed, for the Level E example the results using either the correlation between inputs and the outputs or the standardized regression coefficients shows little (if any) difference. Noteworthy is that one observes at 10^5 years a change in the parameter regime.

4.3.2 Variance-based indices

Variance-based techniques apportion the output variance to the contributions from various input parameters. The main tool is a decomposition of the simulator model into a sum of functions that are orthogonal with respect to the marginal input probability measures. This decomposition is called functional analysis of variance (ANOVA). The output variance can then be distributed among all these functions. Here, each function uses only a subset of the input parameters. The variance explained by a dependence on a univariate function (e.g., of parameter X_j) is called main effect, while the residual variance remaining after removing the variance contributions from functions that do not depend on X_j is called the total effect. Normally, these effects report the relative amount of variance explained with respect to the total output variance. However, in a time-dependent setting, when the output variance is changing over time, it might be advantageous to report the absolute variance attributed to the parameters. Main effects may be estimated using univariate regression curves. Higher order effects can be obtained from fitting regression surfaces, one can approximate total effects by summing first and second order effects (e.g., random-sample high-dimensional model representation (RS-HDMR) uses bivariate products of orthonormal sets of polynomials). Simulation-based methods which require special sample designs are the Sobol' method and the Fourier Amplitude Sensitivity Test (FAST) method, for

estimating first and total order effects. Variants to obtain subset and superset importance (Liu & Owen 2006) and Shapley effects (Goda 2021) are also available. The variogram sensitivity (VARS) method (Razavi & Gupta 2016) offers an approach which interpolates between the Morris elementary effects and the Sobol' total effects.

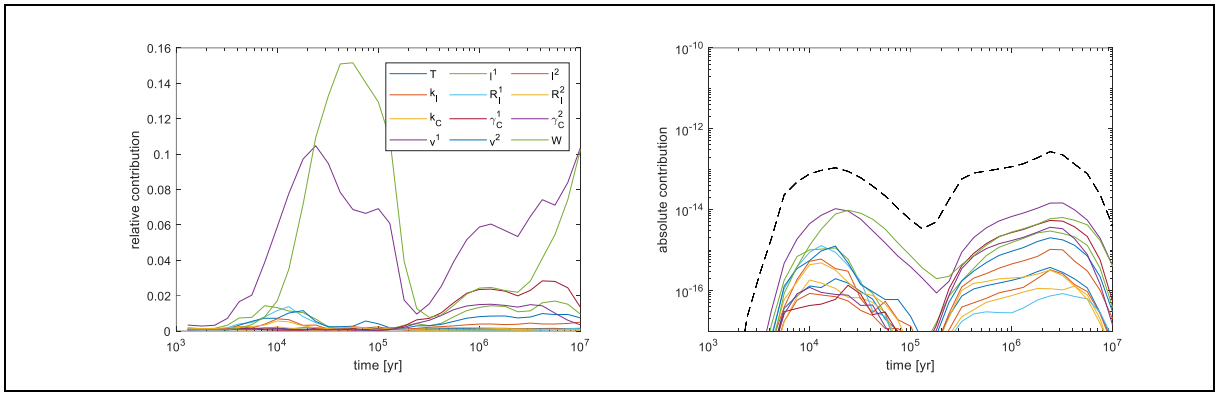

Figure 7 – Time dependent variance-based first order effects for the Level E example. Left: relative contribution to output variance. Right: absolute contribution to output variance (the dashed line represents the time-dependent output variance).

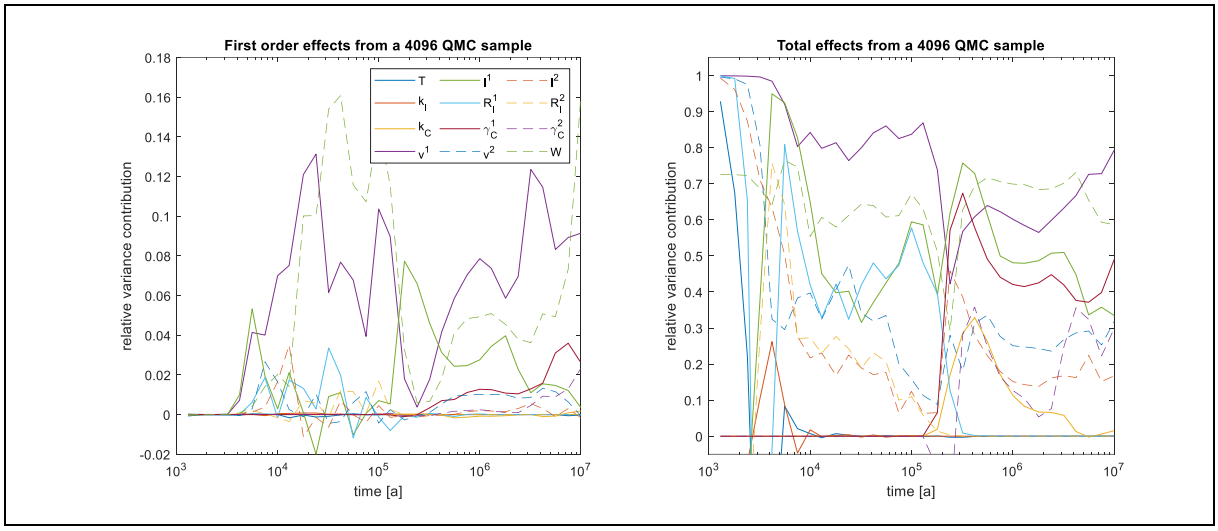

Figure 8 – Sobol' method: Time dependent variance-based first order effects (left) and total effects (right) for the Level E example.

Figure 7 shows the results when first order effects are computed via a data-driven approach. For time-dependent output, the variance may also change with time. Hence the relative variance contribution should be augmented with a plot of the changes in variance, or it should be replaced by the absolute contribution to variance. For a simulation-based method, *Figure 8* demonstrates the outcome of the Sobol' method, with first order and total effects. Despite the relative large sample size (with n(d+2)=57344 simulations, compared to 8192 used for *Figure 7*), no clear picture emerges. The regime shift from iodine-dominated decay to neptunium chain products is visible more prominently in the total effects in *Figure 8 (right panel),* as the sensitivity of iodine retention R_I^1 (light blue) is replaced by the decay chain retention factor γ_C^1 (red) when passing $2 \cdot 10^5$ years. A recent experiment conducted by Puy et al. (2022) on the related PSACOIN Level 0 geosphere transport model shows that including up to third order effects in the sensitivity analysis is not enough to explain the variance to a large extent. Especially methods that use the sum of first and second order effects as a proxy for total effects, e.g., RS-HDMR, are therefore bound to fail on this example.

4.3.3 Moment-independent sensitivity measures

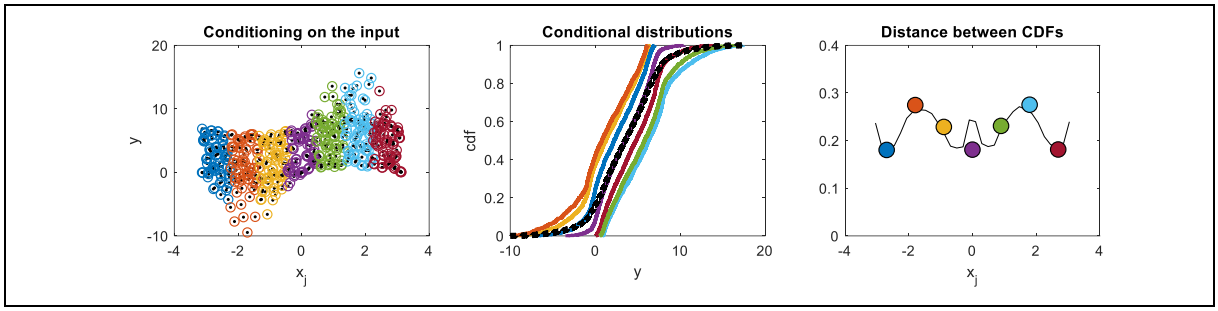

Figure 9 – Data-driven moment independent importance measures: Averaging over all distances gives the sensitivity value for the parameter under inspection (not all points are shown in the left panel, the distance curve in the right panel is extracted from a finer partition).

If variance is not an appropriate measure of uncertainty, then one might be tempted to extend the analysis to higher conditional moments (skewness, kurtosis). However, one normally encounters numerical issues when dealing with large powers putting heavy weights on outliers. Therefore, such a method is not a robust approach. In a more general setting, one can compare the average distance of the unconditional output distribution to the conditional output distributions given that an input parameter is fixed. This value then answers the question of what is gained on average if one receives information that X_i is located at x_i. As there are many ways of defining a distance (between point estimates, cumulative distribution functions (cdfs), probability density functions (pdfs), quantile functions, characteristic functions), this is a rich family of sensitivity measures. If one takes as a distance measure the range in the cdf differences, the Kuiper measure is obtained. *Figure 9* demonstrates the given data technique for obtaining estimates in this framework (Plischke et al. 2013). First, one partitions the input of interest into (color-coded) bins. Second, one derives a cdf from the output data in the bin. Third, computing the distance to the unconditional cdf (dashed line in the middle panel obtained from all data points in the left panel); and finally averaging over all distances. The Kuiper measure, among others, is a transformation-invariant measure, i.e., changes in small output values receive the same attention as changes in large values. This might not be a suitable choice for a risk-based performance indicator. However, with a distance plot (as the right panel in *Figure 9*) and with the sensitivity of specific output quantiles one obtains more localized information. Note that the conditional distance between the properties of unconditional and conditional output probability measures is a random function of the parameter of interest. Statistical measures apart from forming the mean may also be studied, the PAWN method (Pianosi & Wagener 2015) suggests median or maximum as alternatives.

The Level E example shows that the Kuiper measure identifies different key drivers of uncertainty compared to linear or variance-based methods. Especially, the influence of the biosphere parameter *W* is not as prominent as in the variance-based context. This might be due to the Kuiper measure being transformation-invariant, giving the same weight to parameters influencing the output at low and at large values. This might not be the information needed in a risk-based context. In contrast, considering the sensitivity of the 80% quantile of the output (upper right panel in *Figure 10*), reassures us about the findings from the variance-based analysis, demonstrating the large impact of the biosphere parameter as well as the water velocity in the first layer of the geosphere on the upper quantile of the model output.

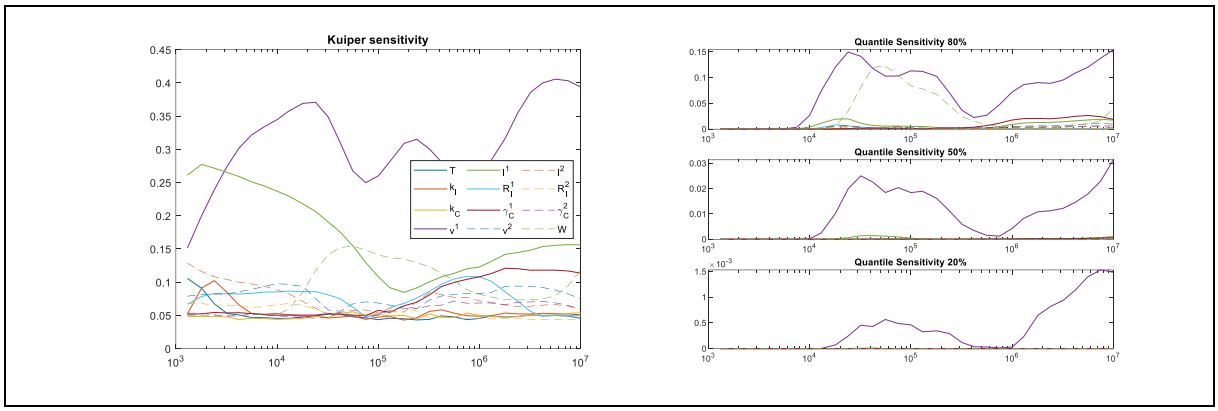

Figure 10 – Moment independent importance measures: Left panel, Kuiper sensitivity. Right panels, quantile sensitivity for the 80% (upper), 50% (middle), 20% (lower) output quantile.

The distance in the moment-independent sensitivity measures $\mathbb{E}\left[d\left(\mathbb{P}_Y, \mathbb{P}_{Y|X_i}\right)\right]$ can be induced by a reproducing kernel in a Hilbert space. Then, under further conditions on the kernel, ANOVA-like decompositions are available. This readily generalizes to multivariate outputs, see Da Veiga et al. (2021).

4.3.4 Graphical tools for sensitivity analysis

For communicating results, graphical representations offer a good compromise between complexity and compactness. Identifying patterns in scatterplots is one of the driving forces behind the development of sensitivity analysis procedures (Kleijnen & Helton 1999). For time dependent data, horsetail plots showing empirical conditional cumulative distribution functions have been suggested. The following methods condense the information of several scatterplots into multiple curves. The contribution to the sample mean (CSM) plot (Saint-Geours et al. 2015) and its modification, the cumulative sum of the normalized reordered model output (CUSUNORO) curve (Plischke 2012), provide information on the behaviour of the conditional sample mean, while CSV studies the contribution to the sample variance, i.e., considering the second central moment. Kendall plots (Genest 2003) are nonparametric: they compare the bivariate empirical input/output copula to the independent product copula, considering one input per curve. Conditional cobweb-plots (also called parallel coordinate plots) may help in visualizing regional information. In interaction plots, an interaction between parameters can be identified by observing non-parallel or intersecting curves.

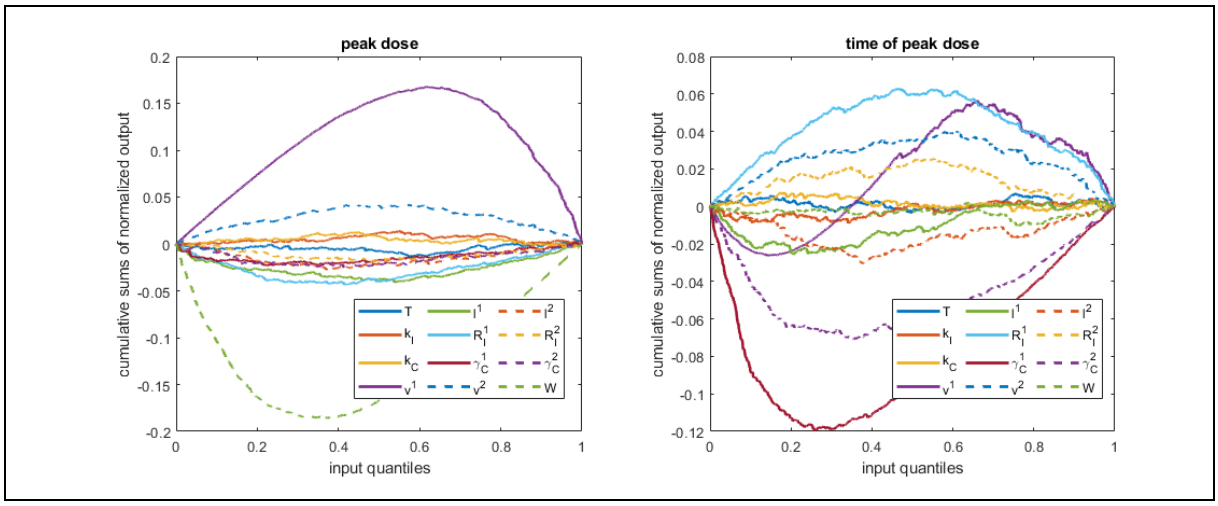

Figure 11 – Cusunoro plots for different quantities of interest. Left: peak dose. Right: time of peak dose.

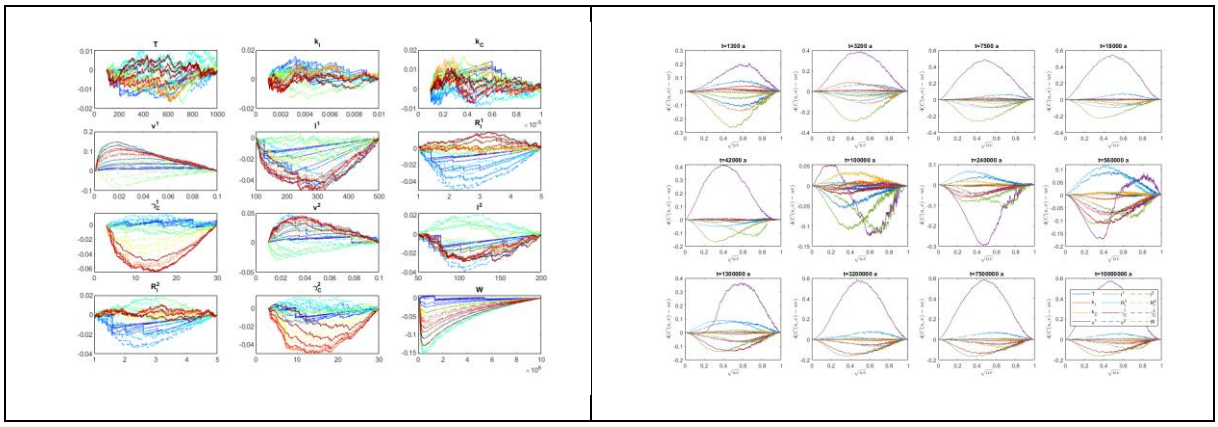

Figure 12 – Time-dependent plots. Left panel: cusunoro plots per parameter (blue: early, red: late times). Right panel: modified Kendall plots per time-step.

Figure 12 demonstrates different techniques for handling time-dependent inputs, organizing the plots either by parameter or by time-step. In this example, both types of plots signal co/contra-monotonic dependence by positive/negative curves. If this is not the case, some nonlinear/nonmonotonic behaviour is expected. This is especially prominent for parameter 4 (v^1) (violet curves in the right panel) where there are three time-steps which do not show a clean positive trend (in the left panel, these are the yellowish-green curves in the v^1 plot). Further parameters with a non-monotonic dependence are the parameters of the second geosphere layer (v^2, l^2,R_I^2,γ_C^2).

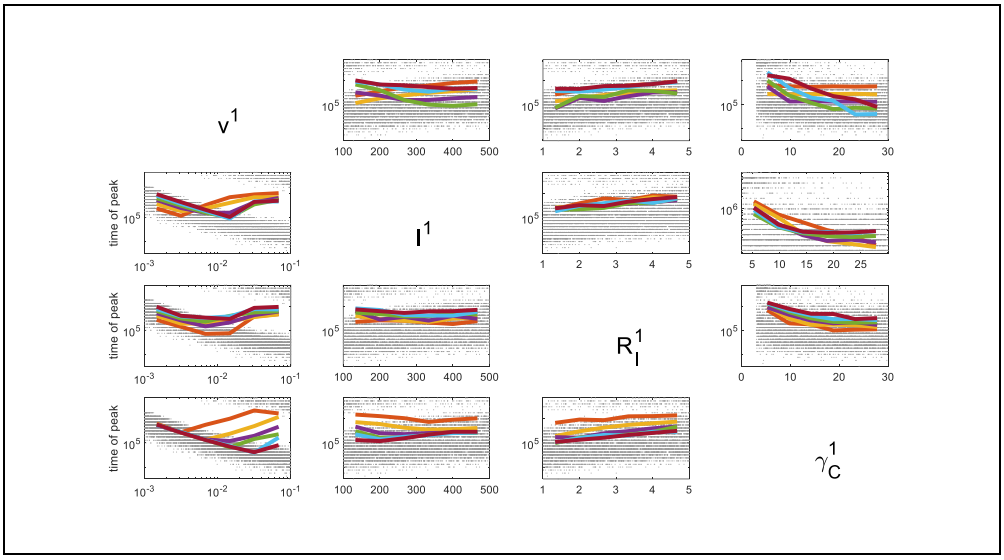

Figure 13 – Interaction plots: Vertically, scatterplots depending on the parameter named on the diagonal are shown, while horizontally one considers conditional means by partitioning on this parameter.

Interaction plots are an approach to tackle parameter interactions. In *Figure 13*, parameters of the first geosphere layer show pronounced interactions (as the curves intersect) when using time of peak dose as quantity of interest.

Other visual methods expand the idea behind regression curves, notable tools are partial dependence curves, individual conditional expectations (ICE) and accumulated local effects (ALE) plots, see Friedman (2001), Goldstein et al. (2015) and Apley & Zhu (2020).

4.4 Further Topics and Open Questions

Further discussions and topics on sensitivity analysis are found in Borgonovo (2017). Computer code implementations of sensitivity methods are discussed in Da Veiga et al. (2021). Python subroutines are available through Iwanaga et al. (2022).

There are open issues with respect to sensitivity analysis. Most methods assume that the input distributions are statistically independent. However, there are examples for an interdependence that cannot be described with an analytical functional dependence, e.g., the relation between porosity and permeability. The application of Sobol' methods then requires a conditionally independent sampling scheme. These methods have not reached maturity in terms of robustness. With the presence of dependence in the input, the interpretation of the higher-order effects changes: It is no longer true that these effects are only due to interaction in the model, they may as well be already present in the input sample.

Techniques for dealing with time-dependent or spatial-temporal output other than introducing a quantity of interest are not widely available at present. The current practise of reporting a variance-based index per time-step needs careful interpretation, as the output variance, being the reference value for the relative sensitivity measures, may change over time. Moreover, in modelling one observes discontinuities, induced by effects as container and seal failures or by transport phenomena before, during and past the transit of a contaminant plume. Changes in the geochemical conditions may also lead to changes in the model behaviour, activating and deactivating different reaction pathways. For the sensitivity analysis of rare events, one might think of combining importance sampling with sensitivity methods. However, there is currently no generally accepted approach.

5. Input from the Questionnaire

The UMAN subtask 2 questionnaire is published in D10.3 (Brendler & Pospiech 2022). Here we comment on the answers to the questions targeting answers regarding the methods applied for uncertainty and sensitivity analysis.

For Uncertainty Analysis, one finds four answers that comment on projects describing the output uncertainty via quantiles, moments, or histograms. Three indirect answers mentioning Monte-Carlo simulation and probabilistic models also demonstrate that the uncertainty in the input or output is modelled probabilistically. Two answers consider deterministic bounds on the output and conservative cases. Seven answers mention none or unclear techniques for uncertainty analysis.

Different techniques in use may also reflect the status of the programme. A more mature modelling approach may be combined with a more detailed uncertainty analysis. The further a programme progresses, the clearer the parameter, modelling and scenario uncertainties should become. Epistemic uncertainties may be reduced by improved system knowledge.

For Sensitivity Analysis, the questionnaire allows multiple answers regarding the methods used. We find eight projects using variance-based methods, seven using linear and rank linear methods, two using graphical methods. A project is also analysed using non-parametric methods. Four answers provide no or unclear information on how sensitivity analysis is handled in their organization. A conclusion to draw from these answers is that variance-based sensitivity methods are used on a routine basis. Moment-independent approaches lack a common software support, hence the willingness to invest into these methods is low.

To exploit synergy effects, let us also report on the findings from the JoSA exercise (Swiler et al. 2021). A working group has been established to investigate existing sensitivity analysis methods and examine new methods with a focus on the use of sensitivity analysis in case studies involving geologic disposal of spent nuclear fuel or nuclear waste. Further goals of the exercise were to gain a better understanding of the strengths and weaknesses of various SA methods, identify cost vs. performance trade-offs of the methods, and highlight best practices and lessons learned.

This exercise studies data sets from repository simulations of different origin, and performs sensitivity analysis on them. It is mainly a data-driven exercise, employing both direct and meta-modelling approaches. Linear, variance-based, moment-independent and visual techniques were successfully put to work. In summary, they found that estimates of first order variance-based indices are easily generated from observational data (i.e., not generated by prescribed sampling schemes) using a variety of approaches. This forms one of the main SA approaches. Linear and rank correlation coefficients and regression approaches continue to be used and are informative. More care needs to be taken when estimating and interpreting moment-independent sensitivity indices, which mostly provide a consistent interpretation which the linear or variance-based indices.

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