ON THE SELECTION OF A METHOD ALLOWING TO EVALUATE THE SENSITIVITY OF A MODEL TO ITS PARAMETERS WITHIN THE SAFETY ASSESSMENT OF RW DISPOSAL FACILITIES

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The paper proposes a methodology enabling the selection of a method for parameter sensitivity assessment during numerical model development and its parametrization. Sensitivity analysis is considered essential for uncertainty analysis, which is provided for under relevant international guidelines on the safety assessment of RW disposal facilities, as well as federal rules and regulations in the field of atomic energy use. The paper provides some case studies on the application of the proposed approach.

Keywords: *radioactive waste, numerical model, uncertainty, sensitivity, safety assessment.*

Introduction

The safety of radioactive waste (RW) disposal facilities is demonstrated taking into account a large number of different scenarios describing certain external impacts and the internal evolution of the system over a long-term perspective. This kind of an analysis requires some predictive estimates that can be done using purpose-developed models of relevant processes [1, 2]. Thanks to the advancements in the IT sector and numerical simulation methods more and more complex models can be created, which, on the one hand, can provide as much as possible detailed description of physical and chemical processes involved, and on the other, requires more input information (parameters). In this case, no absolute accuracy in the parameter values can be attained; and any model is viewed as a simplified description of a studied process based on certain assumptions. Therefore, the simulation result is always characterized with some uncertainty.

The uncertainties associated with the simulations supporting the safety demonstration process should be evaluated: this requirement is stated under international recommendations on the development of models used to assess the state of the environment in the vicinity of nuclear facilities [3, 4], as well as in international [5—8] and Russian regulations on the safety assessment of RW disposal facilities [9—12].

Assessment of model sensitivity is viewed as an important component of the uncertainty analysis performed to identify the dependences between the output result uncertainty and the influence of a specific input parameter. In other words, it helps to understand relative importance of each specific parameter for the model [13]. Sensitivity assessment is mentioned as an integral part of uncertainty accounting process in the recommendations on the RWDF safety demonstration [11, 12].

Even though the sensitivity assessment is considered as an important aspect of model development [3, 4, 14], some case studies from various subject areas demonstrate certain problems in its practical implementation, which were noted in the appendices [15]. Basically, such problems are associated with the use of statistically incorrect techniques that can distort the model uncertainty and sometimes in a quite severe way. Thus, for example, many modelers confuse the assessment of model uncertainty (robustness) with the sensitivity assessment. Also, among developers and users of calculating and predictive software tools, the term sensitivity assessment of a model to its parameters is perceived as an estimate focused on the changes in the output value when the input parameter is varied around a certain value, i. e., local sensitivity. However, such an assessment has some important flaws, which, provided all its apparent clarity, complicate the interpretation of the result obtained. Firstly, the assessment depends on the value around which the variation occurs, or it requires some assumption stating that with respect to the parameter, the partial derivative of the result should be considered constant over the entire region. Secondly, it appears absolutely incorrect in case of nonlinear models. This attitude has evolved historically, since initially the sensitivity analysis was basically reduced to the analysis of the model quality — availability of a large local sensitivity to any input parameter provided an unreasonably high forecast uncertainty, which was perceived as a poor model quality.

Due to the increased focus placed on the modelling uncertainties [16], sensitivity analysis methods with a substantiated mathematical base allowing the consideration of the input parameter variability within the entire range of possible parameter values (global methods) and their development also became increasingly relevant [17].

To date, a fairly large number of global methods has been developed to assess the sensitivity of models to their parameters. Most comprehensive reviews on this topic are given in [18—22] also providing some comparisons of methods based on a different mathematical basis [23, 24]. However, based on these data it's not always easy to draw relevant conclusions about the advantages and disadvantages of a particular method.

This study basically proposes an approach to the selection of a method that could be used to assess the sensitivity of computational and predictive models in a correct way. Therefore, this paper considers the main tasks of sensitivity assessment, as well as the classification of the most common methods applied in this regard according to different criteria.

Criteria for the classification of the sensitivity assessment methods

[17] formulates two basic tasks for the sensitivity assessment (ranging and screening), which most of the specific practical issues addressed by the researchers can be reduced to, such as: which factors essentially affect the modeling result uncertainty due to the lack of knowledge or is there a factor (or a group of factors) the influence of which on the model result uncertainty can be neglected, or which group of factors is responsible, for example, for 70 % of the uncertainty in the modeling result, or is it possible to specify a group of factors, the refinement of which would significantly reduce the result variability, for example, by 90 %.

Input parameter *ranking* or prioritization allows to rank them in accordance with their contribution to the uncertainty of the simulation result, i. e., it is used to identify those parameters, the refinement of which would reduce the uncertainty associated with the result obtained.

Screening or latching allows to identify those input parameters the contribution of which to the uncertainty of the output result can be considered as negligible. Thus, these parameters can be settled at some reasonable value and not accounted for, for example, under the parameter calibration procedure.

Based on the analysis of data from [13, 19—21], sensitivity assessment methods can be classified according to the following criteria: local — global, qualitative — quantitative, the playout type (one-at-a-time — all-at-a-time), as well as the computational complexity. Table 1 provides the definitions for all of the above criteria. As noted above, local methods are limited in their application to the local stability of a model and its assessment; no generalized estimates regarding the parameter relevancy are possible. As noted in [13], quantitativeness and "all-at-a-time" playout type (AAT) are considered as the preferred qualities of a method.

Overview and classification of sensitivity assessment methods

Methods developed and used to assess the sensitivity of a model to its parameters mostly suggest that the theoretical basis can impose certain requirements on the model properties. If they are not complied with, incorrect results may be obtained.

Based on the evaluated publications from various subject areas [15], it was demonstrated that local perturbation methods are most commonly applied in practice. The reviews [19—21] considered a wider range of methods that have found their application.

Table 1. Main characteristics for the classification of sensitivity assessment methods

Local	Global
Considers the output variability depending on the input parameter type around some $\bar{x}$ value, which should be calculated for each input parameter respectively.	Considers the input parameter type within the entire region of variability. Accordingly, it is required to set the definition domain for all the input parameters. If this area is poorly known, the findings should be perceived with caution.
Qualitative	**Quantitative**
Sensitivity is represented by visualization: it is either a presentation of the model results given different parameter values or purposely drawn diagrams (tornado diagram, scatter diagram, posterior distribution of input parameters).	Each factor is associated with a quantitative estimate of its relative influence usually presented via a series of sensitivity indices.
One-at-a-time (OAT)	**All-at-a-time (AAT)**
Output variations are caused by changes in one parameter while all others remain constant.	Output variations occurring due to relevant changes in all of the parameters at the same time, thus, the sensitivity to each parameter is governed by the direct influence of this factor and the joint influence due to the interaction of the factors.
Computational complexity (C)	
Depends on the required number of the computational model runs: $C=k{\cdot}M$, where k is the approximate number of model runs per parameter, M is the number of variable parameters	

The foundations of these approaches and the potential of their application is discussed below.

According to the common perturbation method, input parameters of a model are varied (perturbed) around their nominal value once at a time with relevant estimated effect of this variation on the model result obtained. Thus, this is the case of a local sensitivity assessment.

A global extension of the perturbation method is the Morris method suggesting that a series of output value perturbations is calculated with several input values of the variable parameter being shifted [25]. Two sensitivity indicators are calculated for each of them: the first one allows to assess the overall effect of a parameter change on the change in the result and compare it with the influence of other parameters, and the second one is responsible for the influences of higher orders, i. e., a nonlinear influence or an influence depending on the interaction with other parameters.

Correlation methods for sensitivity assessment suggest that the indices are plotted and ranked according to a correlation analysis of input/output pairs. These methods are correct either for linear or nonlinear, but monotonic dependences between the model output and the parameter. The most famous among the correlation indices are:

- Pearson's correlation coefficient and partial correlation coefficient;
- Spearman's rank correlation coefficient and the partial rank correlation coefficient.

The regression method is also applicable only in case of a linear relationship between the input parameter X_i ($i=1,\dots,M$) and the model output (y), i. e., when regression approximation is possible: $y=a_i+b_iX_i$. Standardized regression coefficients are used as sensitivity indices for the parameters, which can be calculated using the below expression:

$$S_i = b_i \frac{\sigma(X_i)}{\sigma(g)}, \qquad (1)$$

where σ is the standard deviation.

Variational methods used to assess the sensitivity of a model to its parameters are based on the following idea: if the model uncertainty is described by a full variation of its output result (V), then the sensitivity index reflects the contribution of each input parameter to it, i. e., they provide a quantitative assessment of the model sensitivity to the parameters.

Mathematically this approach is based on the variance analysis (also often referred to as ANOVA, from the English ANalysis Of VAriance) [26], which assuming the independence of parameters, allows to expand the variation in a series:

$$V = \sum_i V_i + \sum_{i<j} V_{ij} + \sum_{i<j<m} V_{ijm} + \dots + V_{123\dots M}, \qquad (2)$$

where V_i is the individual contribution to the variation of the output result of the i-th parameter, and V_{ij}, V_{ijm}, etc. up to $V_{123\,\dots\,M}$ are groups of factors. These contributions can be calculated using the below formulas [17]:

$$V_i = V_{X_i}\left(E_{X_{\sim i}}\left\{y \middle| X_i\right\}\right),\ V_{ij} = V_{X_iX_j}\left(E_{X_{\sim i}X_{\sim j}}\left\{y \middle| X_i, X_j\right\}\right),$$

$$V_{ijm} = V_{X_iX_jX_m}\left(E_{X_{\sim i}X_{\sim j}X_{\sim m}}\left\{y \middle| X_i, X_j, X_m\right\}\right) \text{ etc.,} \qquad (3)$$

where E is the average value; V is the variation; subscript stands for the variation of this parameter; the subscript with a wave stands for the variation of all parameters at a constant value of the indicated one.

To solve the parameter ranking problem, the first-order indices S_i^T are sufficient: these indices refer to the direct contribution of the parameter V_i: $S_i^T = V_i / V$. However, the first-order indices cannot provide correct solution to the screening problem (identification of parameters with a negligible effect on the result uncertainty), since they do not consider the potential joint influence of parameter groups on the output variation (formula (2)). To account for parameter interaction, the total-order indices referring to the estimated sum of all components of the series (2), in which the parameter is present, can be used. The total order index can be presented as:

$$S_i^T = \frac{E_{X_{\sim i}}\left[V_{x_i}(y \mid X_{\sim i})\right]}{V} = \frac{V_i^T}{V}. \qquad (4)$$

The zero S_i^T value is a necessary and sufficient condition demonstrating that the considered factor does not produce any influence on the simulation result.

The variational approach to the sensitivity assessment is implemented via the calculation of the Sobol indices [26, 27]. Also, an approximation of the first-order indices can be obtained via a method based on the generalization of the Fourier expansion for the y output (Fourier Amplitude Sensitivity Test — FAST) [28] with its extended version (eFAST) also allowing to calculate the full-order indices [29].

As it come to the main limitation of variational methods: these are based on an assumption suggesting that the variation (second-order statistical moment) of the output is a valid estimate of the model result uncertainty. This assumption is true only if the distribution function of the model output is similar to the normal distribution. If the distribution function of the model output is multimodal or is characterized by a high asymmetry factor (the statistical moment accounts for one third of its order), then the output variation cannot be considered as a correct description of the uncertainty.

In case of such models, one can apply the sensitivity assessment methods based on the calculated influence of parameters on the changes in the distribution function or the probability density function of the output result. In this case, model sensitivity to its parameter X_i can be measured by the distance between the unconditional (f_y) output probability density and the conditional one referring to a parameter held constant at the nominal average value ($f_{y|X_i}$) [19, 21, 22, 30]. The output probability density can be expressed through the integral of the deviation function:

$$S_i = \int_{R^{[G]}} D_g\left[f_y \,||\, f_{y|X_i}(\cdot|X)\right], \qquad (5)$$

where $D_g(P_1 \,||\, P_2)$ stands for the g-divergence function between two probabilistic values (P_1 and P_2).

The simplest task is to compare the conditional (with a constant parameter value) and unconditional cumulative distribution functions. This approach was proposed under the PAWN method [24, 32, 31]. The Kolmogorov - Smirnov (KS) statistics is used as a measure of the discrepancy between the distribution functions:

$$S_i = \underset{X_i}{stat}\left[KS(X_i)\right] = \underset{X_i}{stat}\left[\max_y \left|F_y(y) - F_{y|x_i}(y \mid X_i)\right|\right], \quad (6)$$

where $F_y(y)$ is the unconditional cumulative distribution function of the model output; $F_{y|X_i}(y)$ stands for the conditional cumulative distribution function at a constant parameter value X; $\underset{X_i}{stat}$ is the selected measure (mean, median, etc.).

Index (6) is an absolute measure and its value falls in the range (0.1), i. e., it provides a quantitative sensitivity assessment.

Table 2 and Figure 1 summarize the results of a comparison between different methods used to assess the sensitivity of a model to its parameters. Table 2 summarizes the limitations of the methods providing relevant requirements for the model. Figure 1 presents the classification of sensitivity assessment methods according to such characteristics as computational complexity, playout type, problem to be solved and type of assessment.

Table 2. Sensitivity assessment methods and limitations for their application

Sensitivity assessment method	Model requirements
Pearson Correlation and Partial Correlation	Linearity
Spearman's rank correlation and partial rank correlation	Non-linearity is acceptable, but only in case of monotonicity
Regression coefficients	
Variational methods	The output distribution function can be described by the moments of the 1st and 2nd order (close to the normal distribution)
Maurice method	–
Distribution function methods	

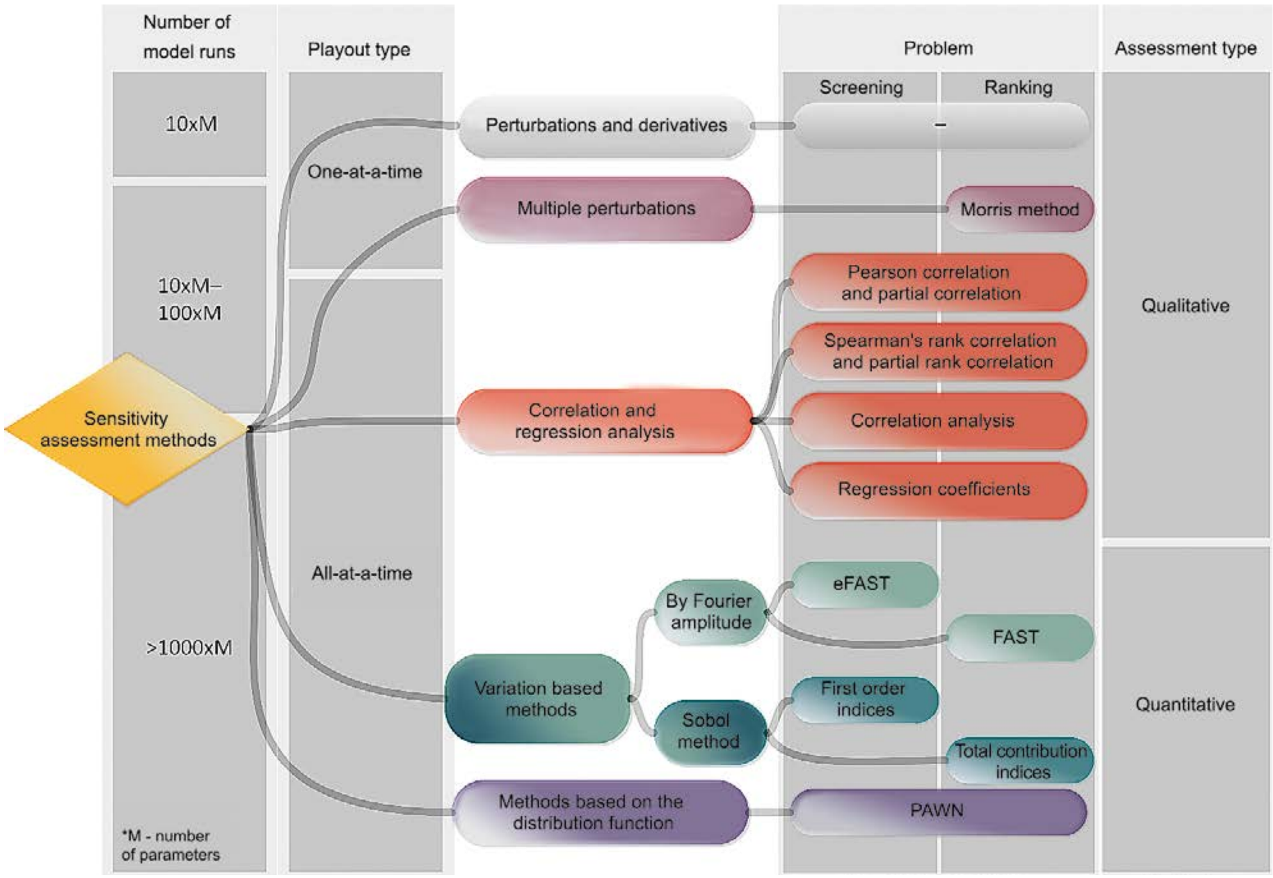


Figure 1. Classification of sensitivity assessment methods

A flowchart enabling the selection of a method for the assessment of a model sensitivity to its parameters

To select a sensitivity assessment method, one should consider the following aspects:

- the potential for its application to address the problem at hand (ranking or screening);
- the computational complexity of the algorithm that implements the method;
- theoretical limitations of the method and, as a consequence, the correctness of its application as regards the considered model.

Thus, the procedure providing the selection of an appropriate method for the assessment of a model sensitivity to its parameters requires the following steps:

- setting the problem as a question related to the assessment of model sensitivity and reducing it to a basic problem (ranking or screening). At this stage, methods that can't solve the basic problem should be excluded from consideration;
- formulation of a priori knowledge about the properties of the model or a series of modeling results;
- if one model run requires some long computation time (depending whether parallel calculations are possible, otherwise — more than 10 minutes) and also if, assuming different parameters ($\leqslant 100M$, where M is the number of variable model parameters), only a small series of results is available, but there are reasons to assume the linearity or monotonicity of the model, it is proposed to use simple correlation or regression methods. It is preferable to use rank correlations (Spearman), which can be used correctly in case of a nonlinear, but monotonic dependence on the parameter. If partial coefficients are applied, parameter influence produced jointly with the others can be excluded;
- if it is not known a priori that the model is linear, this can be checked using the R^2 test, that can be expressed as follows:

$$R^2 = 1 - \frac{\sum_{i=1}^{N}\left(Z^{(i)} - \bar{Z}\right)^2}{\sum_{i=1}^{N}\left(\hat{Z} - Z^{(i)}\right)^2}, \quad (7)$$

where N is the number of input parameter iterations; $Z(i)$ is the result of the output value at the i-th parameter iteration; $\bar{Z}$ is the mean value according to the modelling results for $\left(\bar{Z} = \frac{1}{N}\sum_{i=1}^{N} Z^{(i)}\right)$; $\hat{Z}$ is the mean value of the linear model $\hat{Z} = \beta_0 + \sum_{j=1}^{p}\beta_j X_j$ derived from the regression.

The closer the R^2 value is to 1, the more likely is the index value true. Also, the *p*-value is often calculated under the correlation methods: basically, it stands for a probability showing whether, according to the absolute value, the correlation coefficient of random X_i' and y' from an uncorrelated series will be not lower than the correlation coefficient of the parameter X_i and the output of the model *y*. Accordingly, the closer the *p*-value is to zero, the more you can trust this correlation index. When a ranking problem is solved, one can also resort to the Morris method, for which the model linearity is not considered as a must, but in this case it appears more difficult, however, to get a clear interpretation of the results obtained;

- if the model, according to its properties, can be neither considered as linear nor monotonic, then one should choose among variational methods or approaches based on the distribution function. Variational methods require to check whether the assumption regarding the possibility of describing the modelling result uncertainty in the form of a variation is true, which is the case if the distribution of the simulation result can be interpreted as being similar to a normal one. A characteristic property of the normal distribution is that 68.26 % of all its observations always fall within the range of $\pm 1\sigma$ (standard deviation) from the arithmetic mean, 95.44 % — within $\pm 2\sigma$ and 99.72 % — within $\pm 3\sigma$. In addition, the normal distribution should not be a multimodal one: to check it, the centered moment of the 4th order (kurtosis *E*) can be applied:

$$E = \frac{\sum_{i=1}^{N} \left(z_i - \bar{z}\right)^4}{N \cdot \sigma^4} - 3, \qquad (8)$$

where *N* is the size of the series representing the simulation results; z_i is a single simulation result from the series; $\bar{z}$ is the average for a series of simulation results; σ is a standard deviation of the simulation results in a series. Normal distribution has zero kurtosis. If the distribution has 2 vertices (bimodal distribution), then the kurtosis tends to a negative value. A distribution can be considered close to normal if it is established that from 50 to 80 % of all values fall within one standard deviation of the arithmetic mean and the kurtosis coefficient does not exceed two in its absolute value.

- Sobol method is viewed as the preferred one among the variational methods. However, given huge computational costs of the model running, the FAST method (or eFAST depending on the problem type) based on the fast Fourier expansion can be applied since it requires fewer model runs. However, it should be borne in mind that the approximation of the Fourier expansion in the form of a finite series can result in false dependences;
- if the model result does not correspond to the normal distribution, for example, in case of a multimodal distribution or a high level of skewness, then a moment-independent method should be applied (based on the probability density or distribution function, for example PAWN [31, 32]).

It may happen that the model sensitivity is to be assessed on a previously prepared series of data: the results of a certain model run with given sets of parameters, i. e., the sensitivity assessment is performed suggesting that the model is inaccessible. In this case, the sensitivity assessment method is selected with no account taken of the computational complexity of the model, but may depend on the properties of the series (sets of parameters): its size and structure.

Some issues may potentially arise due to the fact that some algorithms implying quantitative methods for sensitivity assessment require some particular structure of the series according to the model parameters and either the provided set should satisfy these requirements or it should provide the opportunities for building a subseries according to the required structure. Some particular structure is required:

- To evaluate the variation indices of the Sobol sensitivity using the Jansen approximation, which implements the most frequently used assessment algorithm [33];
- If the PAWN method is applied, which is based on assessments and comparisons of conditional and unconditional distribution functions of the output parameters. According to the method used to estimate the conditional distribution function the intervals of the input parameters are divided into subintervals, and if the size of the series is small, some intervals with parameter values may appear containing no points at all.

In this case, to select an appropriate sensitivity method, one has to focus on the size and structure of the series considered. If the use of variational and distribution function-based methods is not possible, one should check if correlation and regression methods can be properly used and focus on them or consider the possibility of using metamodels [20], a detailed description of which falls beyond the scope of this work.

Case studies illustrating the selection of an appropriate method for the assessment of model sensitivity to its parameters

This section specifically illustrates the procedure for the selection of a method allowing to assess the model sensitivity to its parameters. Nevertheless, this article does not draw any meaningful conclusions on the models presented.

Modeling the formation of a RW mixture from two SNF batches

The paper [34] focuses on a model describing the formation of a RW mixture from two SNF batches providing the required characteristics of the waste form.

Input parameters:

- weight coefficient (i. e., the RW composition will involve 10 % of SNF from the 1st batch and 90 % of SNF from the 2nd batch);
- cooling time of the 1st batch;
- cooling time of the 2nd batch.

Output values (considering different cooling times):

- total RW activity;
- total energy release from the RW.

The initial data for the model sensitivity assessment are provided in the form of a series involving 108 samples (input parameters — output values). 3 parameters in the input data are considered variable. The series is built according to a flowchart in which 2 parameters remain constant and the third changes: the first parameter takes on 3 different values, the second — 4, and the third — 9. The output values for each set of inputs are provided considering different points in time.

Figure 1 shows that a series of this size (108) is not sufficient to estimate the sensitivity by variational or distribution function-based methods. Therefore, it is necessary to check the feasibility of correlation and regression method application.

The calculated correlation and regression indices are usually supplemented with the data from linearity tests (this is either R^2, then the value should be close to 1, or p-value, then the value should be closer to 0). In this case, the Pearson and Spearman indices could be considered correct only in case of two parameters, and only the partial rank correlation coefficient was found to be correct for all parameters.

According to the calculations, the cooling time parameter for the second batch appears to be of the highest importance (Figures 2 and 3), but for later time intervals the importance of all parameters becomes quite similar.

Leaching process modeling

[35] presents a kinetic model of the magnesium-potassium-phosphorus ceramics leaching accounting for the precipitation of mineral phases:

struvite ($MgKPO_4 \cdot 6H_2O$)

$$MgKPO_4 \cdot 6H_2O\downarrow \rightarrow K^+ + Mg^{2+} + PO_4^{3-} + 6H_2O, \quad (9)$$

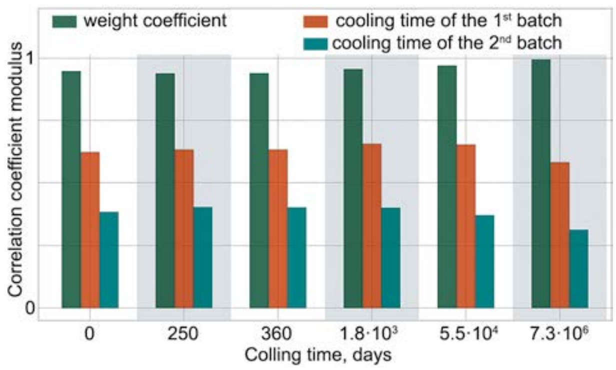


Figure 2. Sensitivity indices (partial rank correlation) for the total activity at different points in time

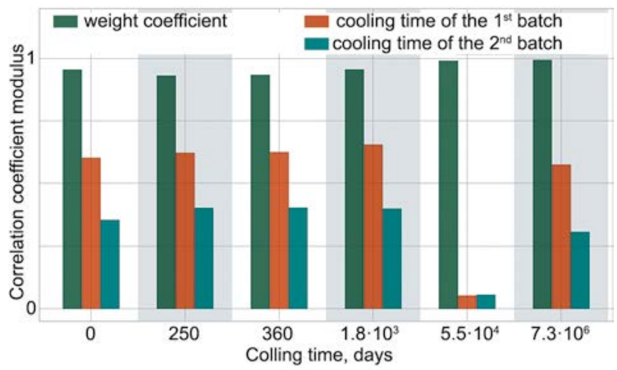


Figure 3. Sensitivity indices (partial rank correlation) for the integral heat release at different times

farringtonite ($Mg_3(PO_4)_2$)

$$Mg_3(PO_4)_2\downarrow \rightarrow 3Mg^{2+} + 2PO_4^{3-}, \quad (10)$$

brucite

$$Mg(OH)_2\downarrow + 2H^+ \rightarrow Mg^{2+} + 2H_2O. \quad (11)$$

Under this case study, estimated was the model sensitivity to the logarithms of the reaction rate constants (9) and (10), as well as the saturation indices of farringtonite and brucite. The calculations ended up with the K, Mg and P leaching curves provided as the output data.

Figure 4 shows the comparison of the regression approximation and the model output, which can be used under the linearity tests. In this case, the nonlinearity of the model is visible considering all three of its input parameters.

The computational complexity of the model is not too high (about half a minute on a personal computer). Therefore, 1,200 runs can be made (if it is possible to parallelize the calculations, this will take several hours). To check if the variational methods can be used for the results obtained, statistical moments were calculated: kurtosis (according to formula (8)), mean and standard deviation to determine the interval "mean ± standard deviation"

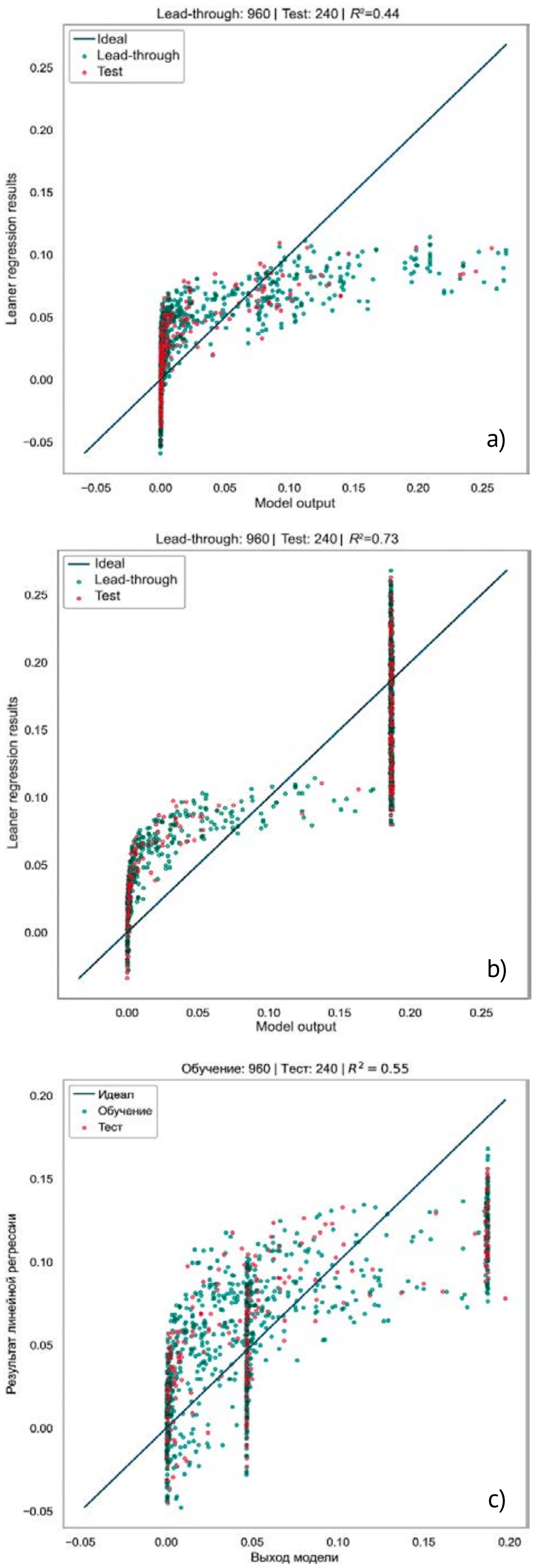


Figure 4. Nonlinearity of the model: linear regression for concentrations of a) Mg, b) K and c) P on the 92nd day

and the percentage of values falling within this range. Table 3 presents the calculated values: it can be seen that only K meets the required criteria: more than 50 and less than 80 % of the simulation results fell into the range of "mean ± standard deviation" values and the excess modulus was < 2. The kurtosis of Mg release is > 2, and in case of P, more than 80 % of the results fell within the “mean ± standard deviation” range.

Table 3. Statistical characteristics of the leaching assessment results

Output	Excess	Interval [mean+std. dev.]	Percentage of points in the interval
Mg	5.5	–	–
P	0.3	[0 ± 0.117]	83.3
K	−1.67	[0.03 ± 0.19]	68.8

Thus, to assess the model sensitivity to its parameters for the K output, it’s considered correct to apply the Sobol variational indices of the first order and the total contribution indices. For other outputs, moment-independent PAWN method can be applied.

To visualize the assessment results from the application of the variational method, different types of representation can be applied.

First-order indices can be represented on a pie chart (for this end they are converted to percentages, see Figure 5a), since their sum shall be less than or equal to 1. If the sum is less than 1, which is immediately visible in the white area, there is a joint influence of groups of parameters, which manifests itself in paired, triple, etc. indices. In the leaching model for the K concentration, a large contribution of the group parameter influence can be observed.

Figure 5b presents the Sobol indices of the first order and the total contribution with the confidence intervals used in relevant assessment considering the same output (K concentration). Confidence intervals can be estimated because the input parameters of the model are considered as stochastic variables, and in the output space, the results of the model implement some distribution being similar to normal. The total contribution indices are used to identify the parameters, the influence of which can be neglected, since they consider the total contribution of a factor, including the one that manifests itself in the interaction with other parameters. In this case, the saturation index of farringtonite is viewed as a parameter not affecting the output: as regards the sensitivity index, the width of its confidence interval practically overlaps its value.

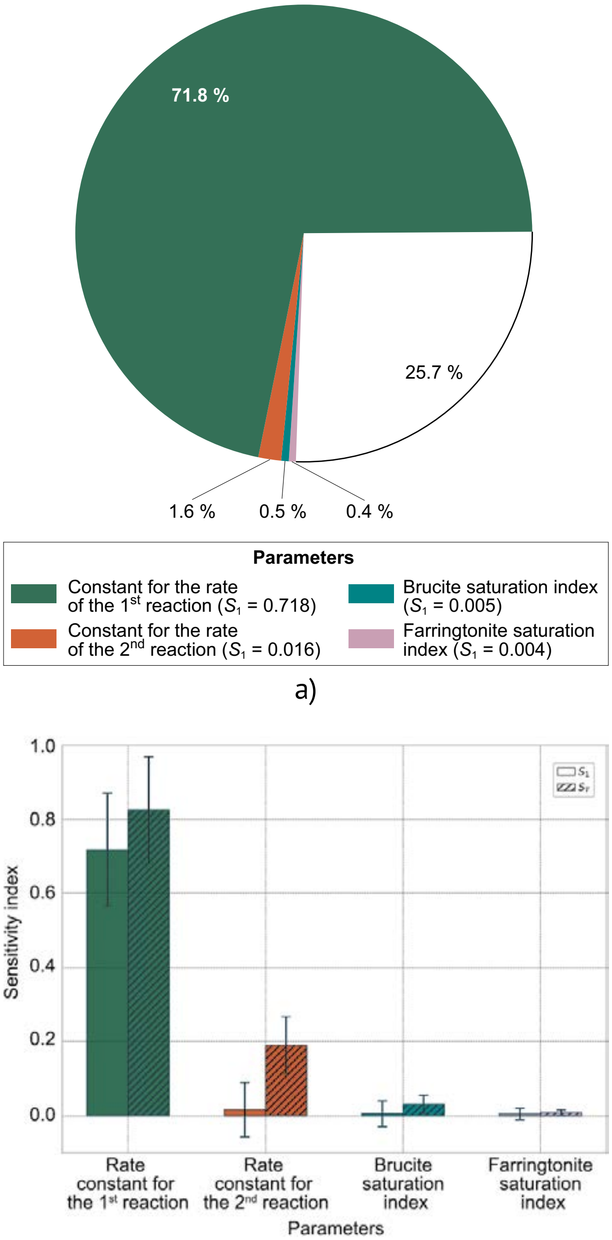


Figure 5. Sensitivity analysis by the Sobol method for K concentrations on the 92nd day: a) indices of the 1st order; b) 1st order and total contribution indices

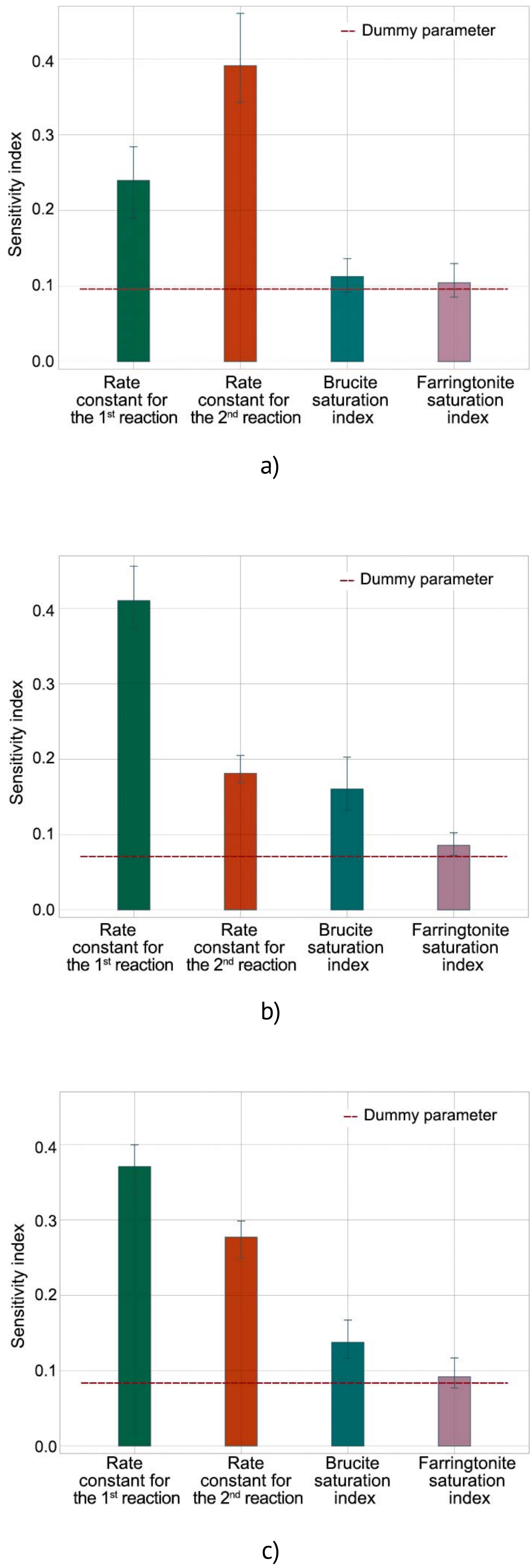


Figure 6. PAWN sensitivity analysis accounting for the concentrations of a) Mg, b) K and c) P on the 92nd day

Figure 6 shows the PAWN sensitivity analysis for all three outputs of the leaching model. It can be seen that the rate constant for the 1st reaction can be considered as the most important parameter for the Mg concentration, and for the other two outputs it accounts for the constant of the second reaction. For the K concentration, it can be also noted that the parameter importance ranking is similar to that obtained using the Sobol method (Figure 6b). Moreover, for all outputs, the farringtonite saturation index amounts to some dummy parameter level (obviously not being able to produce any effect).

Overflow probability evaluated for the terminal reservoir of the Techa cascade of reservoirs (TCR)

The model is designed to assess the overflow probability for the terminal water body of the TCR, as well as the accident probability (when the level of the maximum allowable 90Sr specific activity in the channel of the Techa river is exceeded) [36].

Based on the graphs presented in Table 4, one can conclude that the dependences between the model outputs and the input parameters are nonlinear and not always monotonic, and that the distribution function can be characterized by multimodality and/or asymmetry. Thus, neither correlation and regression nor variational methods can result in a correct model sensitivity assessment. Therefore, one should fall to a method based on the comparison of the distribution functions (PAWN).

Figure 7 presents the sensitivity indices calculated by the PAWN method. Since this method can yield in biased estimates, the use of a dummy parameter [23] was proposed to determine the magnitude of this bias. This parameter was artificially introduced into the analysis and, by definition, could not influence the result. However, in case of approximations or due to some issues associated with the applied pseudo-random number generator, the sensitivity index of the model to such a parameter can still turn out to be greater than zero. The sensitivity index of the model to the dummy parameter (red line in Figure 7) can characterize the approximation error.

Each sensitivity index in Figure 7 is accompanied by a confidence interval: it can be seen that in case of parameters 1—3 from Table 4, the lower confidence interval level is located above the dummy line for both outputs, i. e., these parameters affect the simulation result, and in case of the last two parameters, even the upper confidence interval level is below the dummy line, which means that the model dependence on these parameters can be neglected.

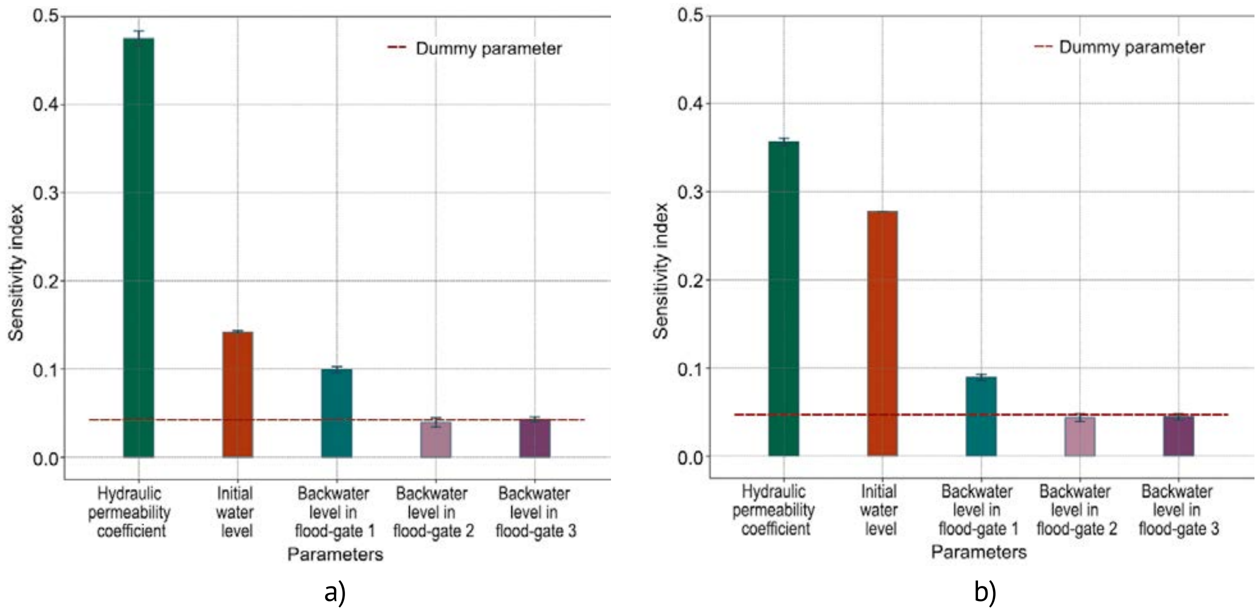


Figure 7. PAWN sensitivity analysis for a) the probability of an accident and b) the probability of the reservoir overflow

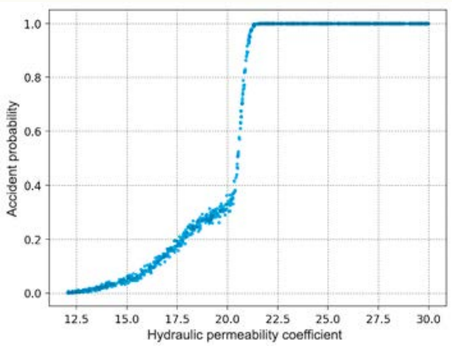
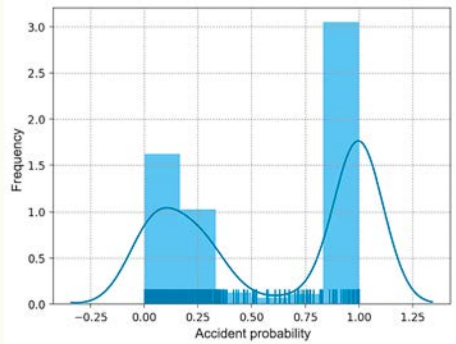
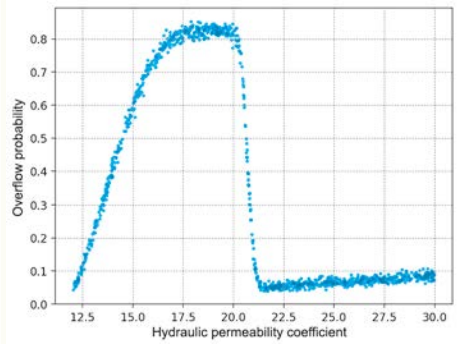
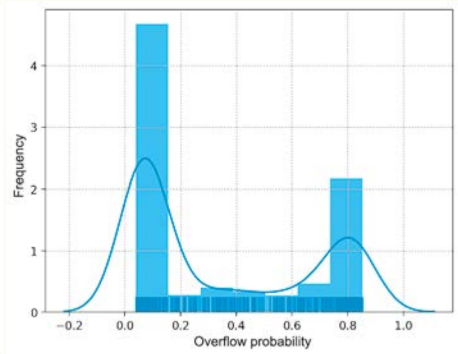
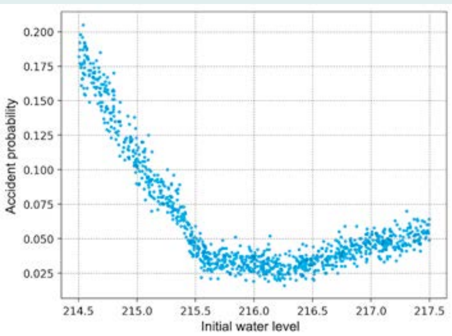
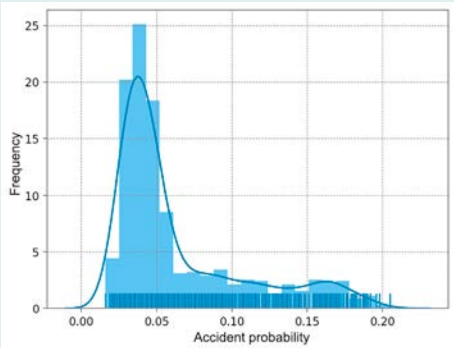
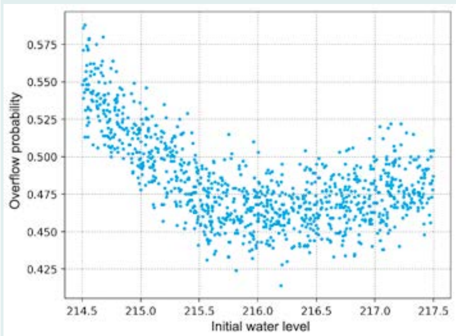
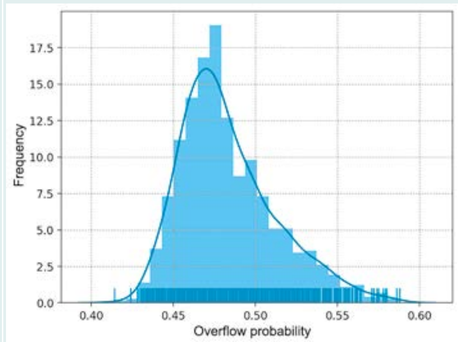
Conclusions

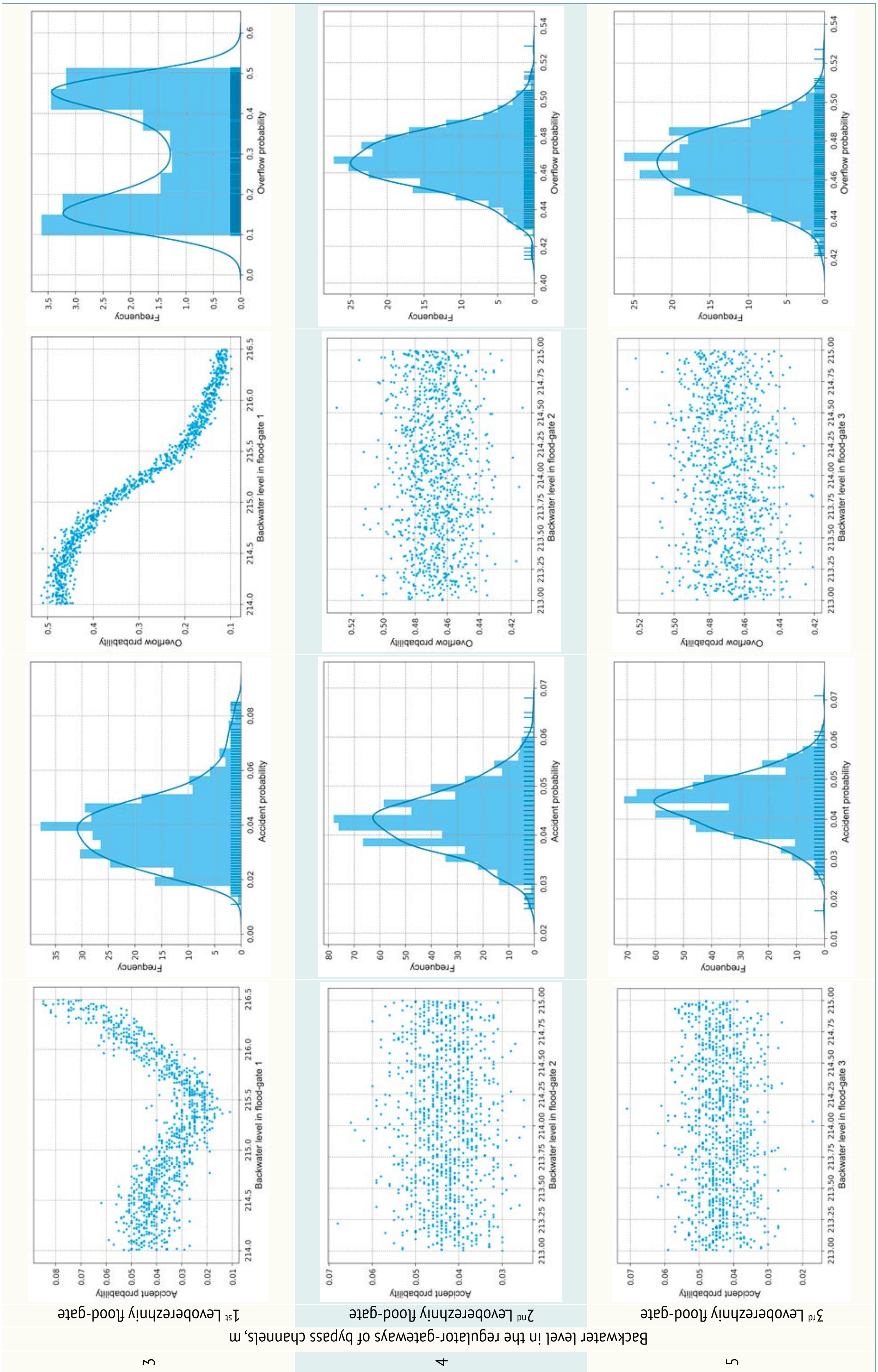
Sensitivity assessment of a computational model is seen as a useful tool providing the segregation of the model input parameters depending on how the uncertainty of their values contributes to the uncertainty of the simulation result. Accordingly, one can select those parameters, the refinement of which would most dramatically reduce the uncertainty in the result, as well as those that considering their contribution can be specified simply according to the data from a reference book.

The number and the variety of methods proposed for the sensitivity assessment of a model to its parameters makes it difficult to select an appropriate method that would result in correct estimates needed by developers and users of computational and predictive models and being non-experts in the field of mathematical statistics. Therefore, in most cases, they use the methods that intuitively seem to correspond to the considered problem, which in fact is far from always being the case.

This paper proposes a classification of sensitivity assessment methods according to the features being considered important in terms of their practical

Table 4. Dependence of the TCR model outputs considering variations in one parameter with other parameters being viewed as constant

No	Parameter	Accident probability		Probability of an overflow	
		Dependence	Probability density	Dependence	Probability density
1	Hydraulic permeability coefficient for the Levoberezhny bypass channel, m/day				
2	Water level in the V-11 reservoir by the time when the calculations were started, m				


3
4
5
Backwater level in the regulator-gateways of bypass channels, m
1st Levoberezhniy flood-gate
2nd Levoberezhniy flood-gate
3rd Levoberezhniy flood-gate
Accident probability
Backwater level in flood-gate 1
Backwater level in flood-gate 2
Backwater level in flood-gate 3
Frequency
Overflow probability

application. A procedure describing how an appropriate method can be chosen was proposed as well. It is to a greater extent based on the developer's understanding of the model than of the methods used. The paper also provides relevant case studies discussing the application of the proposed procedure.

The developed and proposed methodology providing the selection of a sensitivity assessment method can be considered as a groundwork for the development of appropriate methodological recommendations on the sensitivity assessment of models used in the safety assessment of RW disposal facilities.

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