UDC: 621.039.75

VARIATION APPROACH TO SENSITIVITY ASSESSMENT OF A MIGRATION MODEL

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Article received on February 12, 2019

The article deals with the sensitivity assessment of the migration model to the filtration and migration parameters of engineered barriers and geological environment. The pollutant starts moving from the radioactive waste disposal facility and moves towards the river through the a crack. Modeling and sensitivity assessment were performed for two different concepts of the disposal facility. The problem of sensitivity assessment is formulated as a selection of a ed set of parameters, the exact knowledge of which will reduce the uncertainty of the modelling result by 90%.

Key words: *pollutant transfer modelling, sensitivity, uncertainties, safety assessment, radioactive waste disposal.*

Introduction

Calculation and predictive modeling is viewed as an important part of long-term safety demonstration performed during RW disposal facility siting process. Such modeling is aimed at obtaining model estimates showing whether system elements implement their safety functions or not. This is done given the inevitable presence of various types of uncertainties [1].

Modern numerical models account for a large number of factors defining individual characteristics and processes, thus, requiring a large number of input parameters. Sufficiently accurate knowledge is available hardly for all of these parameters in advance: to refine some of these, additional field or laboratory studies are required. As for the others, due to limitations of measurement methods or their natural variability, they may contain some ineliminable uncertainties. Nevertheless, to obtain modeling results, all parameters must be specified in one way or another with some of them requiring a higher level of accuracy. That is why special attention is paid to the fact that modeling should be accompanied by an assessment of relevant calculation model showing its sensitivity to changes in its parameters, as well as estimation of uncertainties associated with calculation result. This is stated both in regulatory documents [1] and international practice on the review of safety cases developed for final RW disposal facilities [2].

Sensitivity analysis allows a multilateral assessment of the influence produced by input parameters on the modeling result. This enables to avoid further consideration of the input data not affecting or just slightly affecting the result, group parameters influencing correlatedly and etc. during parameter optimization and characterization of uncertainty. Moreover, sensitivity assessment might be helpful in comparing different engineering solutions.

This paper presents a case study showing how a modification of a variation approach is applied to sensitivity assessment for a model describing radionuclide transfer in a geological environment. Model sensitivity to the parameters characterizing it is demonstrated, as well as the important influence that most important parameters adopted in the model have depending on the engineering solutions provided for in deep RW disposal facility designs.

Sensitivity analysis method

Assessment of model sensitivity to its parameters is commonly applied in its classic formulation suggesting that the input parameters are ranked based on the degree of their influence on the changes in the output values [3].

Importance of a parameter can also be estimated by its contribution to the variation of the output result: the most important is considered a parameter whose fixation on the true value ensures the minimum variation of the output result. Such an understanding can be conveniently interpreted in solving risk assessment problems with limited initial data available due to insufficient knowledge: it is precisely these model parameters are identified the refinement of which can result in a reduced variation (in other words, the uncertainty) of the simulation result.

The main difficulty is that the true value of the parameter is unknown. Thus, a good approximation to the above formulation may be seen not in fixing the parameter on the true value, but considering it as a mathematical expectation in a certain distribution, i.e. fixed averaging. In this case, most important input parameter will be the one that being fixed, on average, provides the maximum reduction in the result variation.

Let us introduce the following notation: $X=\{X_i\}$, $i=1,\ldots,$ N — vector of model input parameters, Y — output modeling result. X_i parameter averaging fixation over its entire distribution when calculating the variation for each fixed value stands for $E_{X_i}\left\{V_{X_{\sim i}}(Y\,|\,X)\right\}$, where E_{X_i} is averaging over different values of Xi parameter, $X_i, V_{X_{\sim i}}$ — variation with all parameters except for X_i being varied. The smallest $E_{X_i}\left\{V_{X_{\sim i}}(Y\,|\,X)\right\}$ or, as a result, the largest value $V_{X_i}\left(E_{X_{\sim i}}\{Y\,|\,X\}\right)$ is identified by this very factor. It means that, to solve a problem under such a setting for the uncorrelated and non-interrelated parameters, variational sensitivity index (S_i) can be applied [3]:

$$S_i = V_{X_i}\left(E_{X_{\sim i}}\{Y\,|\,X_i\}\right)\big/V(Y), \tag{1}$$

where $V(Y)$ is full result variation.

The issue associated with lacking parameter correlation should be considered separately — sensitivity analysis always ensures correct results if correlations are absent. To check whether such interactions are really missing, the following equation may be applied:

$$\sum_j V_j = V(Y)\,. \tag{2}$$

When relation (2) is fulfilled, all variables can be ranked depending on the index value from formula (1) showing their contribution to the output variation:

$$S_{R_1} \ge S_{R_2} \ge \cdots \ge S_{R_N}, \tag{3}$$

and, thus, to identify the most significant ones.

If relation (2) is not fulfilled, we cannot decisively select the first rated variables, since they can participate in the joint effect and screen the importance of other variables. The interaction of two variables is described as:

$$V_{ij} = V\left(E\left\{Y\,|\,X_i, X_j\right\}\right) - V\left(E\left\{Y\,|\,X_i\right\}\right) - V\left(E\left\{Y\,|\,X_j\right\}\right) \tag{4}$$

Similar formulas can also be identified to present the interactions of a higher order, and the general form of variation decomposition can be expressed as a sum [4, 5]:

$$V = \sum_i V_i + \sum_{i<j} V_{ij} + \sum_{i<j<m} V_{ijm} + \cdots + V_{123\ldots N}\,. \tag{5}$$

Variation approach applied for ranking model parameters by their importance rate is implemented in various software designed for sensitivity assessment: SAFE [6], SimLab [7], DAKOTA [8]. The latter was developed by Sandia National Laboratories (USA) and is recommended by the IAEA to perform sensitivity and uncertainty assessments. Its implementation within the framework of a software complex being developed by Nuclear Safety Institute (IBRAE RAN) is also provided for sensitivity and uncertainty assessment purposes [9].

However, the variation approach can be used for a slightly modified problem, namely: to identify such model parameters the refinement of which reduces the variation in the result by a given percent, for example, by 90% [10]. Thus, the target value for reducing the variation (V_{tar}) should be defined as $V_{tar}/V(Y) = 0.1$. If there is no mutual influence of variables, r first variables in the ranking will provide a solution to this problem, so that:

$$\sum_{i=1}^{r} V_{R_i} \ge V - V_{tar}\,. \tag{6}$$

To perform such a sensitivity assessment, in the absence of interactions between variables, the Morris method [11] can be used. This method involves estimation of first-order variations, that is, an apparatus enabling to calculate V_i.

But in general case that doesn't go far enough to solve such a problem — consecutive evaluation is needed: first, the contribution of each variable should be assessed, then the effects of each couple followed by triplet interaction evaluation and so on. A most common option suggested to solve this problem provides for the use of Sobol indexes being considered precisely as the estimates of a variation for sets of variable groups [4, 5].

To perform relevant calculations, an algorithm was proposed suggesting the use of a full index of model sensitivity to a parameter. Full index (V_{T_i}) stands for a component of a sum (5) elements of which contain members related to this parameter X_i accounting for an average variation of the result given the uncertainty of the studied parameter $\left(E\left\{V(Y \mid X_{-i})\right\}\right)$. Parameters the refinement of which allows to reduce the variation of the result by 90 % are identified based on the following procedure:

1) Full set of V_i indexes is calculated, V_i, $i = 1,\ldots,N$ and V_{T_i}, $i = 1,\ldots,N$ ..

2) Variables are ranked according to V_{T_i} values with a following sequence obtained: $V_{T_{R1}} > V_{T_{R2}} > \cdots > V_{T_{RN}}$.

3) Parameter with the highest overall rating index is selected (*R1*). If $V_{R1} > V - V_{tar}$, then the problem is solved — exact knowledge on X_{R_1} parameter will reduce the output variation by 90 %, otherwise, the procedure is followed up to step 4.

4) Parameter with the second highest overall index (*R2*) is selected, if $V_{R1} + V_{R2} + V_{R1R2} > V - V_{tar}$, then parameters X_{R1} and X_{R2} are selected. If not, the procedure is followed up.

5) Parameter with the remaining highest overall index ($X_{T_{Rk}}$) is selected. Calculated are all pairwise variations $V_{Ri,Rk}$, $i = 1,\ldots,k-1$, triplet variations $V_{Ri,Rj,Rk}$, $i,j = 1,\ldots,k-1$, $i \neq j$ and variations of higher orders to the $k(V^c_{R1,\cdots,Rk})$. If

$$\sum_{j=1}^{k} V_{Rj} + \sum_{\substack{i,j=1\\ i\neq j}}^{k} V_{Ri,Rj} + \sum_{\substack{i,j,m=1\\ i\neq j\neq m}}^{k} V_{Ri,Rj,Rm} + \cdots + V_{R1,\ldots,Rk} > V - V_{tar},$$

then $X_{T_{Rk}}$ is added to the existing set, and the procedure is deemed to be completed; if not, step 5 is repeated.

Below discussed is the application of the described approach in modeling radionuclide transfer in the geological environment.

Description of models and variable parameters

A number of engineering options suggesting different borehole designs are proposed for the borehole disposal of RW containers. This paper focuses on two different options: open-end and dead-end boreholes. The boundaries of the model are shown in Fig. 1. Open-end boreholes are boreholes connecting horizontal excavations at two operational levels (Fig. 2), whereas, dead-end boreholes are isolated by rock from the side of a horizontal excavation (Fig. 3). It's assumed that 75 m deep vertical boreholes having a diameter of 1.3 m will be located at a distance of 15 m from each other with each borehole containing 18 insulating containers with radioactive waste. Modeling result should enable to evaluate the amount of conventional pollutant released into the river over a period of 10,000 years.

The calculated area for the case of open-end boreholes consists of 18 wells and 2 tunnels with a nearby crack spreading towards the river (Fig. 2). The case of dead-end boreholes considers 1 tunnel and 18 wells with a crack marked in red (Fig. 3).

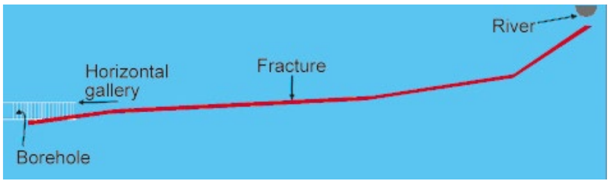

Fig. 1. Model boundaries

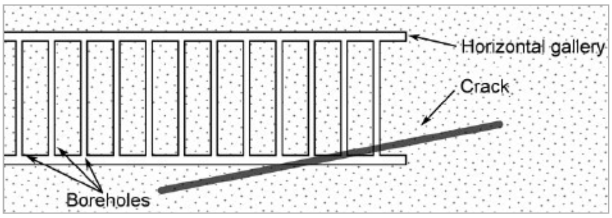

Fig. 2. Layout of dead-end boreholes

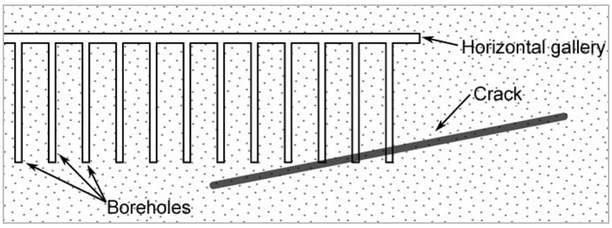

Fig. 3. Layout of open-end boreholes

Pressure gradient was calculated for two boreholes with the distance between them amounting to 2,000 m and a pressure drop of 50 m. The resulting gradient accounted for 0.025. Ranges of parameter variation (table 1) were identified with due account of the rock mass heterogeneity based on the following considerations:

- The range for rock filtration coefficients for virgin formations was selected based on the measurements made during geological surveys [12];
- A wide range was assumed for the filtration coefficients of rocks located in fractures as it is often difficult to assess the filtration properties of fractures when studying the geological properties of

Table 1. Variable model parameters

Parameter	Description	Range of values
Kf_rock [m/day]	Filtration coefficient for virgin rocks	0.00001–0.0048
Kf_tun [m/day]	Filtration coefficient for horizontal galleries with man-caused fracturing (tunnel)	0.01–0.3
Kf_bor [m/day]	Filtration coefficient for vertical boreholes with RW packages	0.001–0.1
Kf_fract [m/day]	Filtration coefficient for rocks in fractures	0.0002–0.3
Por_rock	Average active rock porosity	0.33 % (0.3–1 %)
Por_tun	Active rock porosity in the man-caused fracturing zone	5 % (1–20 %)
Por_bor	Active rock porosity in vertical boreholes	1 % (0.5–1.5 %)
Por_fract	Rock porosity in fractures	1 % (0.1–5 %)

a rock mass, since they can be either water-conducting or filled with some matter;

- The range of filtration coefficient variation for horizontal galleries with man-caused fracturing was chosen based on the following assumptions. Drilling and blasting methods will be used to excavate the horizontal galleries potentially resulting in crack formation. Under resulting hydrogeological conditions, water inflow may occur precisely along these potential cracks.
- For vertical boreholes, filtration coefficient range was determined based on rock mass properties, excavation conditions and engineered safety barriers used for RW packages.
- Porosity coefficients were chosen based on literature data, as well as data from [12] and expert evaluations. Filtration and transport processes were simulated using GeRa code [13]. GeRa software is a program designed for three-dimensional calculations of unsteady isothermal filtration and multicomponent transport problems in inhomogeneous and, possibly, anisotropic geological environments. In keeping with the provisions of its certification passport, GeRa provides for prediction and epignosis calculations of the hydrogeological and hydrogeochemical conditions on a local or regional scale.

Filtration problem was solved under stationary pressure setting. To calculate the mass transfer, the initial concentration of the contaminant in each borehole was taken equal to 1. Under pessimistic evaluations, a non-absorbable pollutant was assumed.

Results of the sensitivity assessment

The sensitivity assessment was carried out based on the method described above using Sobol indexes for a relative amount of pollutant entering the model boundaries at the time of 10,000 years. Sobole indexes of the first order V_i, second order V_{ij} and general V_{T_i} were calculated using the SALib library [14] in Python 2.7. The assessment procedure was carried out based on the data provided in Tables 2–5 (indexes are sorted in a descending order, zero and close to zero second-order indexes are not given) and consisted of the following steps:

- The studied models were checked for additivity: for both models, relation (2) is not satisfied, the models are considered as not additive;
- Parameter ranking:
  - For an open-end borehole model, the highest overall index rating was observed for the parameters of well filtration coefficients, horizontal galleries and virgin rocks Kf_bor, Kf_tun, Kf_rock;
  - For a dead-end borehole model, the highest overall index rating was associated with filtration coefficients of virgin rock, fractures and horizontal galleries Kf_rock, Kf_fract, Kf_tun.
- Selection of parameters enabling to reduce the variation by 80 %:
  - For an open-end borehole model, the contribution of a parameter with the highest first-order index (filtration coefficient for naturally-occurring virgin rock Kf_rock) is sufficient to reduce variation by 80 % (table 3);
  - For a dead-end borehole model, a single parameter seems to be not enough. Data from Table 4 evidences that Kf_rock and Kf_fract account for the largest contribution, whereas data from Table 5 provides a clear demonstration to the fact that their joint contribution is sufficient for the desired decrease in the result variation.

Thus, it was demonstrated that for open-end boreholes, filtration coefficient for virgin rock has the greatest impact on the result uncertainty. As for the dead-end borehole model, the important contribution of fracture filtration coefficient should be also taken into account.

Table 2. Result variation and its decrease by 80 %

Open-end borehole model		Dead-end borehole model	
V	$9.17 \cdot 10^{-2}$	V	$35.42 \cdot 10^{-2}$
$V - V_{tar}$ (80 %)	$7.33 \cdot 10^{-2}$	$V - V_{tar}$ (80 %)	$28.34 \cdot 10^{-2}$

Table 3. First-order indexes in a descending order

Open-end borehole model		Dead-end borehole model	
X_{Ri} (parameter)	V_0	X_{Ri} (parameter)	V_{Ri}
Kf_rock	$8.22\cdot10^{-2}$	Kf_rock	$18.99\cdot10^{-2}$
Kf_fract	$1.11\cdot10^{-3}$	Por_rock	$4.86\cdot10^{-3}$
Por_rock	$8.31\cdot10^{-4}$	Por_fract	$2.89\cdot10^{-3}$
Por_fract	$2.4\cdot10^{-5}$	Por_bor	$2.74\cdot10^{-3}$
Por_bor	$1.64\cdot10^{-5}$	Kf_bor	$2.71\cdot10^{-3}$
Por_tun	0	Kf_tun	$1.60\cdot10^{-3}$
Kf_bor	0	Kf_fract	$9.31\cdot10^{-4}$
Kf_tun	0	Por_tun	0
$\sum_i V_{Ri}$	$8.42\cdot10^{-2}$	$\sum_i V_{Ri}$	$20.56\cdot10^{-2}$

Table 5. Second-order indexes in a descending order

Open-end borehole model			Dead-end borehole model		
X_j (parameter)	X_m (parameter)	V_{jm}	X_j (parameter)	X_m (parameter)	V_{jm}
Kf_rock	Kf_fract	$4.90\cdot10^{-2}$	Kf_rock	Kf_fract	$4.43\cdot10^{-1}$
Kf_rock	Por_rock	$3.52\cdot10^{-2}$	Kf_rock	Por_rock	$1.44\cdot10^{-1}$
Kf_rock	Por_tun	$3.10\cdot10^{-2}$	Kf_rock	Por_bor	$1.18\cdot10^{-1}$
Kf_rock	Por_fract	$3.00\cdot10^{-2}$	Kf_rock	Por_tun	$1.16\cdot10^{-1}$
Kf_rock	Por_bor	$3.00\cdot10^{-2}$	Kf_rock	Por_fract	$1.15\cdot10^{-1}$
Kf_tun	Kf_rock	$2.43\cdot10^{-2}$	Kf_tun	Kf_rock	$9.58\cdot10^{-2}$
Kf_bor	Por_rock	$7.63\cdot10^{-3}$	Kf_bor	Kf_rock	$1.34\cdot10^{-2}$
...					

Table 4. General indexes in a descending order

Open-end borehole model		Dead-end borehole model	
X (parameter)	V	X (parameter)	V
Kf_tun	$7.42\cdot10^{-1}$	Kf_rock	1.02
Kf_bor	$7.10\cdot10^{-1}$	Kf_fract	$5.76\cdot10^{-1}$
Kf_rock	$3.52\cdot10^{-1}$	Por_tun	$4.19\cdot10^{-1}$
Kf_fract	$1.57\cdot10^{-1}$	Kf_tun	$2.72\cdot10^{-1}$
Por_rock	$1.25\cdot10^{-2}$	Por_rock	$2.59\cdot10^{-1}$
Por_bor	$2.05\cdot10^{-5}$	Kf_bor	$2.12\cdot10^{-1}$
Por_fract	$1.80\cdot10^{-5}$	Por_fract	$2.10\cdot10^{-1}$
Por_tun	$2.21\cdot10^{-6}$	Por_bor	$2.10\cdot10^{-1}$
$\sum_i V_{TRi}$	1.97	$\sum_i V_{TRi}$	3.18

Conclusion

Understanding the parameters making more important contribution to the result variation is essential in terms of effective accounting of uncertainties. Without such an understanding, it's believed to be impossible to address the safe RW disposal challenge to its full extent, as well as to introduce the resulting knowledge on contaminant spread into safety case materials.

This paper is focused on the application of a variational method to sensitivity assessment to model contaminant transfer in a geological environment.

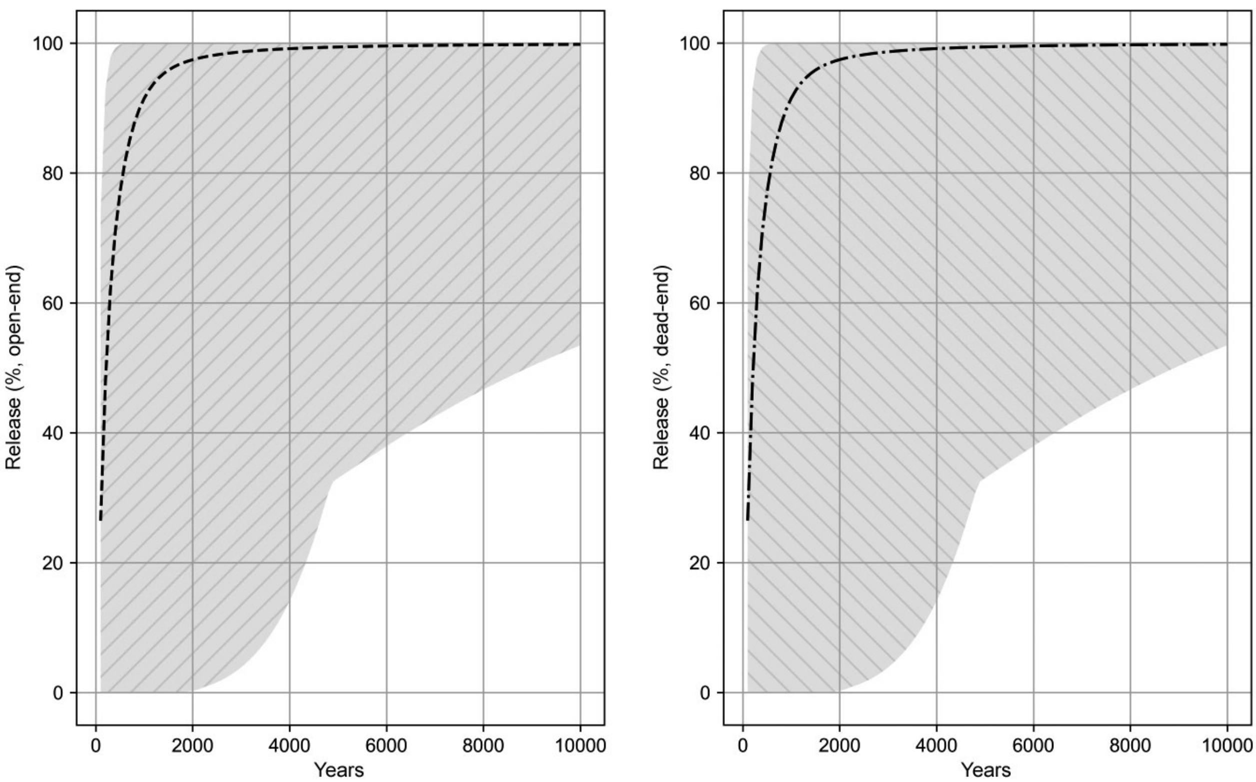

Fig. 4a. Spread of the time dependence showing the portion of contaminant released into the river assuming the initial range of parameters

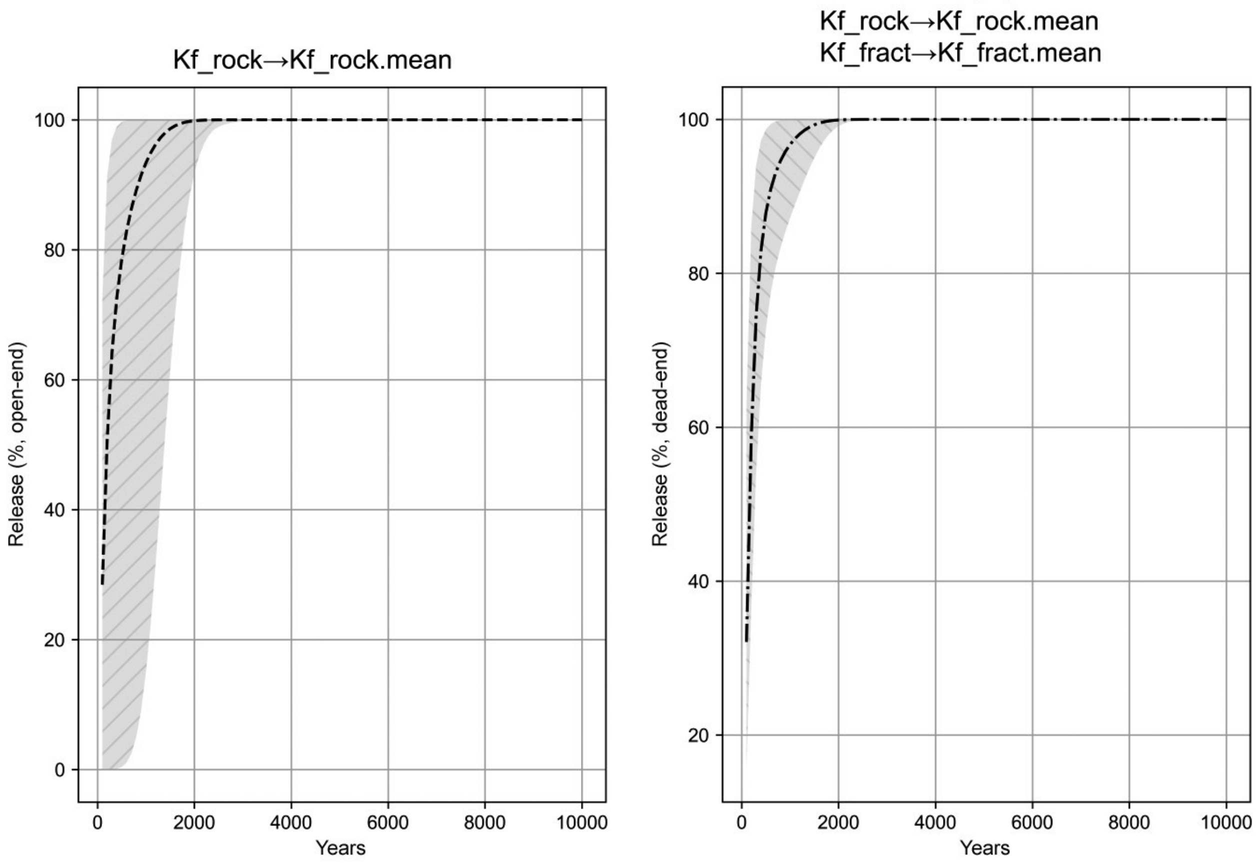

Fig. 4b. Spread of the time dependence showing the portion of contaminant released into the river assuming a fixed set of most important parameters

The analysis performed allowed to conclude that the refinement of such parameters in further studies allows for the greatest reduction of modeling result uncertainty.

Moreover, sensitivity assessment yields the conclusion that depending on the design solutions envisaged for the disposal facility the most important are the parameters characterizing various elements of the geological environment. This is yet another point confirming that the choice of a deep disposal concept impacts on the set of top priority studies to be performed.

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Bibliographic description

Neuvazhaev G. D., Saveleva E. A., Svitelman V. S. Variation Approach to Sensitivity Assessment of a Migration Model. *Radioactive Waste,* 2019, no. 1(6), pp. 69—76. (In Russian).