Hybrid Cuckoo Search and Harmony Search Algorithm and Its Modifications for the Calibration of Groundwater Flow Models

D. K. Valetov[a], G. D. Neuvazhaev[b], V. S. Svitelman[c] and E. A. Saveleva[d]
Nuclear Safety Institute of the Russian Academy of Sciences, Bolshaya Tulskaya Street, Moscow, Russia

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Abstract: Due to inherent uncertainties associated with the groundwater system characterization, the model calibration is the significant step for the obtaining of the reliable predictions that could be used in long-term safety assessment. The following paper is focused on the modelling of the groundwater flow in heterogeneous media using the data of the geological engineering survey for the prospective site of the radioactive waste deep geological disposal at Nizhnekansky granite-gneiss crystalline rock massif (Krasnoyarsk Territory). This case study illustrates the efficiency of heuristic optimization methods and hybridization approach for the calibration of groundwater models.

1 INTRODUCTION

Safety assessments of the prospective radioactive waste disposal are based on models of the disposal facility and of its natural surroundings. Numerical models of radionuclide transport processes in geological media require the set of site-specific parameters like flow and transport properties, boundary conditions and so on. And these parameters are associated with significant uncertainties due to the natural variability of the geological media, lack of the ability to measure them at each point of interest, and the simplifications during the construction of the numerical model.

Model calibration aims to reduce uncertainty in the parametrization of the numerical model by comparing the model predictions with site-specific field observations and measurements. In practice, if a model can be calibrated successfully for a variety of site-specific conditions, it means an increased level of confidence in the model's ability to represent the system behaviour and estimate its effects that cannot be measured.

The model calibration has always been an essential step for groundwater flow and transport modelling, and the approaches and techniques have been developing, evolving and inter-influencing: from the manual calibration through gradient-based and direct search to the heuristic and various hybrid methods. Gradient-based methods are based on the use of local derivative information to guide the search direction and may not achieve an optimal solution in complex problems with a large number of decision variables due to converging to local suboptimal solutions.

The alternatives are to utilize deterministic pattern-based procedures (direct search) or adopt structured randomness elements from natural optimization strategies (heuristic and meta-heuristic algorithms) (Maier et al., 2014). The last ones have been extensively used lately to solve calibration problems in different scientific fields including groundwater flow and transport modelling because they appeared to be able to overcome such common challenges as mixed parameter types, the nonlinearity, the discontinuities and the local minima (Maier et al., 2014), (Haddad et al., 2013).

The problem under consideration in this paper is parametrization of the cross-sectional groundwater flow model in the heterogeneous geological media

[a] https://orcid.org/0000-0001-5432-4084
[b] https://orcid.org/0000-0001-6821-1638
[c] https://orcid.org/0000-0002-5976-6049
[d] https://orcid.org/0000-0002-6562-8750

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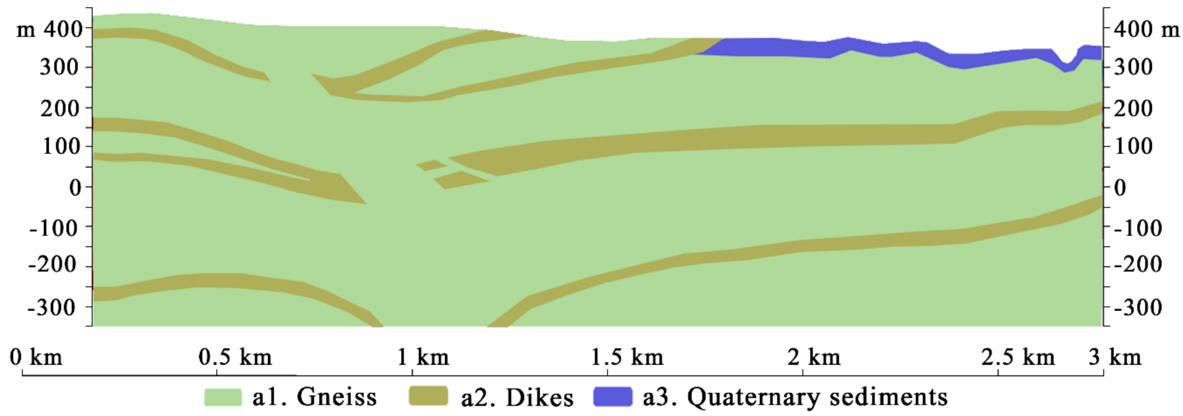

Figure 1: Schematic geological cross-section of the modelling area, model 1.

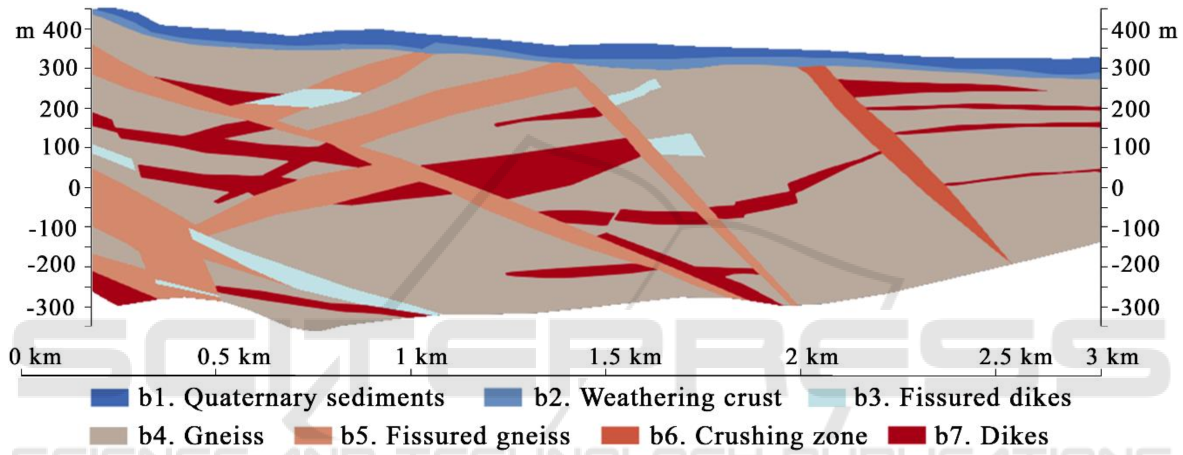

Figure 2: Schematic geological cross-section of the modelling area, model 2.

based on the data of geological survey in the area of the prospective radioactive waste deep geological disposal. The parameter optimization tool used for this model is a hybrid algorithm (Fister, 2015) that combines the advantages of two different heuristic methods. First, Cuckoo search (CS) has great exploratory qualities due to the use of Levy Flight. And the second one, Harmony search (HS), provides efficient exploitation of the search space by efficient adjustment of positions of the search agents. In addition to the existent hybrid, two improvements of it are considered: the use of CS with a chaotic varying step size (Wang et al., 2016) and the modification of the distribution for the HS.

2 PROBLEM DESIGN

Russian deep geological repository project has been started about 30 years ago. To date, the siting procedure is completed, and the license for the construction of the underground research facility (URF) at Nizhnekansky granite-gneiss crystalline rock massif (Krasnoyarsk Territory) is received. The scope and purposes of the URF are site characterization, technology development and testing, safety assessment and demonstration in support of the development of the deep geological disposal. The current concept under consideration of the deep geological disposal is following: two disposal levels will be located at 450-525 m depth. High-level waste containers will be located in deep vertical boreholes. That is consistent with internationally considered mined deep borehole matrix concept (Baldwin, Chapman and Neall, 2008).

During the geological survey of the site the wells were drilled to depths of 700 m, the packer tests with interval pressure measurements and single pumping tests were carried out. The groundwater flow model represents the steady-state problem in the confined media.

The differential equations that describe groundwater flow are the following:

$$\nabla \cdot \vec{u} = Q \tag{1}$$

$$\vec{u} = -K \nabla h \tag{2}$$

where $\vec{u}$ is the velocity vector determined by Darcy law (2) and h – hydraulic head, Q – sources and drains, K – hydraulic conductivity.

These equations are solved by the finite-volume method with two-point flow approximation by means of GeRa groundwater flow and transport modelling computer code (Kapyrin et al., 2018).

The two models have been constructed on the basis of the structural geological cross-sections corresponding to the two alternative interpretations of the well data (Jobmann, 2016) (figures 1 and 2). Different geological structural elements (a1 – a3 for model 1 and b1 – b7 for model 2) are indicated by different colors.

The boundary conditions for each model were set in the following way:

- The right border was drawn along streamlines ending on the Shumikha River (the streamlines from the hydrodynamic point of view are the impermeable boundaries);
- The lower boundary corresponds to no-flow boundary condition due to the fact that the rocks that lie at the mark -350m are treated as impermeable;
- On the upper boundary the rainfall recharge rate was set to 0.00001 m/day, except for the Shumikha River on which Dirichlet-type boundary condition with the level of 331m was set;
- At the left border, Dirichlet-type boundary condition with the constant hydraulic head of 400m was set, which was obtained on the basis of water level measurements.

The hydraulic conductivity coefficients were varied during calibration in the separate range for each structural element (3 parameters for the model 1 and 7 parameters for model 2). Parameter variation ranges were set by expert assessment and given in the Results section. The underlying rationale is the following. For intact rock specimen ranges of the hydraulic conductivities were set according to the geological survey findings (Jobmann, 2016). And for fractured rock (b3.Fissured dikes, b5.Fissured gneiss, b6.Crushing zone) were set wider ranges because fractures could be both water-conductive and non-conductive based on the available information.

Observations for the calibration were represented by 35 known hydraulic heads from 3 pumping wells.

3 CALIBRATION AS OPTIMIZATION PROBLEM

For credible safety assessment of the geological disposal system a model that properly represents an actual system is required. Hence the model calibration procedure aims to obtain a set of parameters that would produce the best possible fit of simulated and available observed values quantified by the target function (Hill, 2004). During this procedure, the vector of model input parameters is varied by a specific algorithm, and the target function (most commonly it is sum of weighted least-squares) is evaluated at each step.

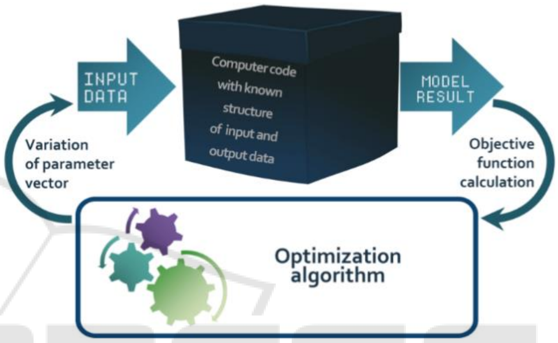

Figure 3: Scheme of the interaction between black box model and optimization algorithm.

Therefore, the calibration is a particular case of the global optimization problem where groundwater flow is represented as a black box with the vector of the input parameter and the target function as the response variable (figure 3). The aim is to find the minimum of target function surface in parametric search space.

Such characteristics of groundwater flow and transport models as nonlinearity, multimodality, the high dimensionality of search space makes the application of the gradient-based methods inefficient for them. These conditions made the use of the heuristic algorithms that combine rules and randomness to imitate natural phenomena very popular. The reason for the variety of heuristic algorithms is explained by «no-free-lunch theorem of optimization» that states that a general-purpose, universal optimization strategy is impossible.

The only way one heuristic method can outperform another is if it is specialized to the structure of the specific problem. The promising way of such kind of specialization is hybrids that combine multiple algorithms in order to employ their advantages and compensate for the weaknesses. It is

Table 1: Adjusted properties of the optimization methods.

Algorithm	Hyper-parameter	Value
Cuckoo Search	Population size (CMS)	20
	Abandon probability (PA)	0.1
	Step size scaling factor (α)	0.25
	Dispersion coefficient for Levy Flight	1.5
Harmony Search	Population size (HMS)	20
	Harmony Memory Considering Rate (HMCR)	0.5
	Harmony Memory Considering Rate (HMCR) (in hybrid algorithm)	1.0
	Pitch adjusting rate (PAR)	0.5
	Step size scaling factor (α)	0.01
Hybrid parameters	Number of Harmony Search iterations to be done per each Cuckoo Search iteration	6
	Chaos map to be used in Chaos Cuckoo Search	logistic
	Dispersion coefficient for distribution used in modified Harmony Search	6.67

worth mentioning that the concept of hybrids can be found in the engineering of nature-based solutions as is the case, for example, in the human brain where applying multiple memory systems guarantees the optimality of decision-making (Hamid and Braun, 2019).

The hybrid algorithm (CS/HS) that combines Cuckoo Search and Harmony Search was proposed by Wang et al. (Wang et al., 2016). The basic algorithm in the hybrid is CS (Gandomi, Yang and Alavi, 2013). The CS algorithm is inspired by the parasitic brood reproductive strategy of cuckoo birds. Specifics of cuckoos nesting process are following: cuckoos lay their eggs in the nests of other birds; the host bird could discover them with some probability (PA) and abandon the nest or throw the alien egg away. In the algorithm each cuckoo is represented by a point in search space, if an egg has not been discovered by the host bird, then it remains and another cuckoo appears at this point. Target function in this metaphor is the quality of the nest (lack of predators, food availability, etc.)

The CS algorithm uses Levy flight search pattern to explore search space. It mimics the behavior that is very common for different bird and insects species: series of straight flight paths punctuated by sudden turns (Cole, 1995), (Rhee et al., 2011). Such characteristics of Levy distribution as infinite mathematical expectation and variation, and power-law tail and positive asymmetry have a positive effect on global search in the search space. Search process with step sampled from this distribution covers the search space faster than if with normal distribution used. Moreover, bell-bottomness of this distribution advances sampling of medium steps and thus better local search too. This optimization method is effectively used for high dimension problems in a wide range of problem fields, including geological modelling problems, for example, underground water resources estimate (Gupta, Das and Panchal, 2013).

To sum up, the hyper-parameters (the options that can customize the algorithm's behavior) are the following:

- population size (Cuckoo Memory Size – CMS);
- probability for an egg to be discovered by host (Abandon Probability – PA);
- step size scaling factor related to the scales of the problem of interest (α);
- dispersion coefficient for Levy Flight distribution (σ) (Cole, 1995), (Rhee et al., 2011);
- step size scaling factor related to the scales of the problem of interest (α).

The second component of the hybrid is HS (Ayvaz, 2009). It reproduces the idealized natural musical improvisation processes. In this metaphor parameter values are pitches of instruments, the target function is the aesthetic standard, and the global optimum is perfect harmony.

The search process includes three components: memory consideration, pitch adjustment, and random selection. Properties of the algorithm are the following:

- amount of harmonies (parameter vectors) in memory (Harmony Memory Size – HMS);
- probability to choose an instrument pitch from memory (Harmony Memory Considering Rate – HMCR);
- the probability to adjust harmony chosen from memory (Pitch Adjusting Rate – PAR);
- step size scaling factor related to the scales of the problem of interest (α).

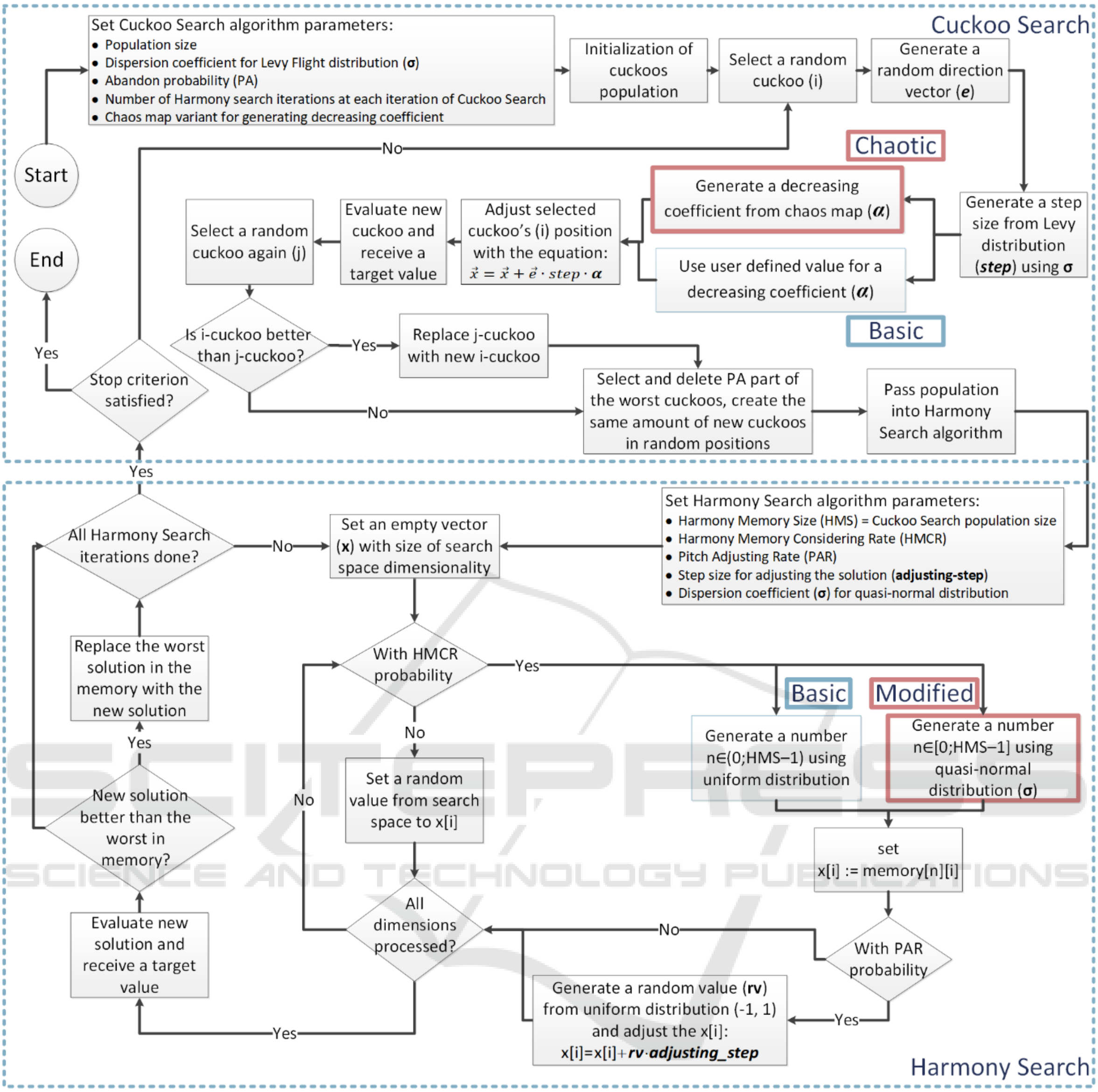

Figure 4: Hybrid CS-HS algorithm.

HS is widely used in medicine and engineering design and in groundwater management problems (Ayvaz, 2009). However, this method has a tendency to population diversity decrease, which leads to sticking at a local optimum.

Hybridization of the algorithms has the form of sequential stages: each Cuckoo Search iteration is followed by several Harmony Search iterations applied to the decisions' population. The right adjustment of the Harmony Search properties has a critical influence on the efficiency of the search. In this work, we propose the particular settings of the hybrid properties that were chosen after consideration of the results of (Wang et al., 2016), and our own tests on the multimodal analytic benchmark problems (Jamil & Yang, 2013). First, HMCR was set to 1.0 to make Harmony Search only to combine new solutions by adjusting or remembering without improvisation. This may quickly degrade the population, thus we set the number of HS iterations not more than the size of the population. This decision is empirical experienced. HS and CS population sizes were set equal. The values of all the properties are listed in table 1.

Alongside the well-known HS/CS hybrid, two improvements for it were considered (separately as well as all at once). The first of them is also a well-known modification by the author of the basic CS method where the constant step size α is substituted by chaotic varying step (Chaotic Cuckoo Search, CCS) (Wang et al., 2016).

This significantly enhances the performance of the CS by chaotically changing the decreasing multiplier using chaotic sampling by a chaos map – section, that was modified can be seen on, the upper red box – where standard α is changed on chaotic α, that is generated on each iteration. This hybrid is referenced in the next section as CCS/HS.

More information on comparison of the performance of the listed methods compared to the classic heuristic algorithms like PSO and GA can be found in (Wang et al., 2016), (Wang et al., 2016), (Yang & Deb, 2009).

The modification to the HS component is proposed by the authors of this work and its core idea is to replace uniform random selection from the memory with the probability HMCR by the selection using modified normal sampling distribution. The sampling steps are: 1) sample a normally distributed value with 0 mean and HMS/3 (experience-based value) standard deviation; 2) take absolute value and discard non-integer part; 3) if this value is more than the size of population – sample a value with uniform distribution in [0, HMS-1] interval. The result value will be the donor solution order number in population. It allows us to use parameters of best solutions more often while combining a new solution to evaluate (population is sorted before constructing a new solution). The hybrid method with modified HS is referenced as CS/MHS. Modification of Harmony Search is marked by the lower red box on.

And the last hybrid under consideration is the combination of both chaotic CS and modified HS: CCS/MHS.

Integral flow chart of described above hybrids is presented on figure 4.

4 RESULTS

The basic hybrid method (CS/HS) and three proposed variants were applied to the calibration of the two groundwater flow models described above. The series of 20 optimizations with random initial populations were performed for each method and each model. The target function for all cases was the sum of squared residuals. The stop criterion for every optimization was: 100 model runs without improvement of the best found target value.

The model parameters, their ranges of variation and the obtained optima results are given in the tables 2 and 3. Geological materials names are presented in the tables 2 and 3 with their pseudonyms from the figures 1 and 2. Models with optimized parameters provided the agreement between the experimental data and the simulation outputs at the observation points with 5% precision. These metrics of the results were quite similar for all four compared hybrids. The obtained values allow making several conclusions. First, the hydraulic conductivity coefficients for element of geological structural model – parts of the same lithology substantially vary with different fracture density. It means that subselection of the geological structural elements with diverse fracture density may be crucial for the quality of simulations. The second finding from the calibration is that slightly fractured dykes are likely to act as natural barriers.

The visualizations of the comparison of the alternative algorithms via convergence plots (Beiranvand, Hare and Lucet, 2017) are presented on figures 5 and 6. The number of model runs is plotted on the horizontal axis and the target function values are on the vertical axis. The lower bound of each filled contour is the convergence curve for the fastest optimization among each method's trials, the upper bound – for the slowest one, and the bright-colored line is the mean. According to the plots, all algorithms appeared to be quite effective for model 1, their mean convergence lines are very similar. Convergence for model 1 is reached by 400-500 model runs. Model 2 required far more (about 10-20 thousand) model runs to converge. And that is hardly surprising because of more detailed parameterization of this model (7 parameters versus 3). And in this case, the effectiveness of the considered algorithms significantly differs. The CCS/HS hybrid converges faster than others.

At first glance, the hybrids with modified Harmony Search (CS/MHS and CCS/MHS) show worse performance than CS/HS and CCS/HS on the average.

On the series of convergence plots for these algorithms (figures 7 and 8), one can see that approximately half of the optimizations converges to the suboptimal decision due to the tendency of the modification to "condense" the decision set.

This ability to stably find not only the best decision but also a set of suboptimal ones should be considered further. In the context of the groundwater flow and transport modelling the inherent uncertainty of the available data is commonly rather significant. And because of that suboptimal parametrization of the model under consideration could be helpful for the uncertainty assessment.

Table 2: Ranges of variation for model 1 parameters and found optimal values.

Material	Hydraulic conductivity coefficients [m/day]	
	Variation ranges	Optimal value
a1.Gneiss	$(1.0{\cdot}10^{-5}; 1{,}0{\cdot}10^{-3})$	$7.43{\cdot}10^{-4}$
a2.Dikes	$(1.0{\cdot}10^{-5}; 1{,}0{\cdot}10^{-3})$	$6.93{\cdot}10^{-4}$
a3.Quaternary sediments	$(1.0{\cdot}10^{-2}; 5{,}0{\cdot}10^{-1})$	$1.16{\cdot}10^{-2}$

Table 3: Ranges of variation for model 2 parameters and found optimal values.

Material	Hydraulic conductivity coefficients [m/day]	
	Variation ranges	Optimal value
b1.Quaternary sediments	$(1.0{\cdot}10^{-3}; 5.0{\cdot}10^{-1})$	$4.998{\cdot}10^{-1}$
b2.Weathering crust	$(1.0{\cdot}10^{-3}; 5.0{\cdot}10^{-1})$	$1.00{\cdot}10^{-3}$
b3.Fissured dikes	$(1.0{\cdot}10^{-6}; 3.5{\cdot}10^{-2})$	$5.21{\cdot}10^{-5}$
b4.Gneiss	$(1.0{\cdot}10^{-6}; 1.0{\cdot}10^{-2})$	$9.06{\cdot}10^{-4}$
b5.Fissured gneiss	$(5.0{\cdot}10^{-3}; 1.0{\cdot}10^{-1})$	$5.001{\cdot}10^{-3}$
b6.Crushing zone	$(1.0{\cdot}10^{-2}; 1.0)$	$1.27{\cdot}10^{-2}$
b7.Dikes	$(1.0{\cdot}10^{-6}; 1.0{\cdot}10^{-3})$	$6.09{\cdot}10^{-2}$

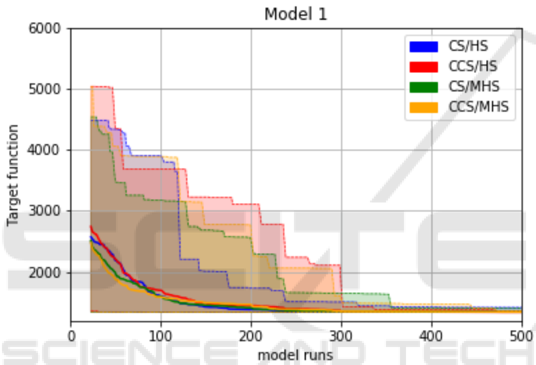

Figure 5: Convergence plots for compared algorithms for optimization, model 1.

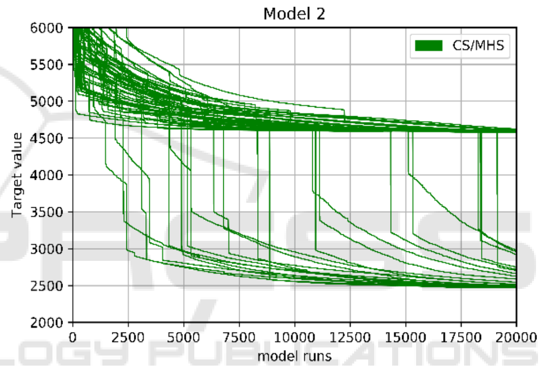

Figure 7: Separate convergence plots for CS/MHS, model 2.

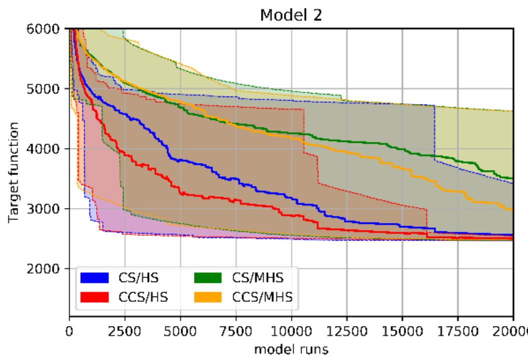

Figure 6: Convergence plots for compared algorithms for optimization, model 2.

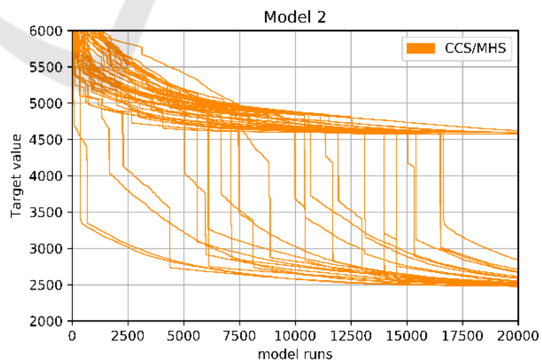

Figure 8: Separate convergence plots for CCS/MHS, model 2.

5 CONCLUSIONS

In this work, the hybrid CS/HS optimization algorithm and its modifications were successfully applied to the calibration of two alternative groundwater flow models on the basis of geological survey data of prospective site of the radioactive waste deep geological disposal. The simulation results obtained with the optimized parameters appeared to be in good agreement with the experimental data and could be used for radionuclides transport simulations that are required as part of long-term safety assessment for this sort of projects.

The combination of the proposed improvements of the basic CS/HS algorithm was found to be reasonable for this case of the optimization problem. Hybrid methods with HMS component should be developed further. And the CCS/HS variant appeared to be the most efficient and stable among the others. These qualities are highly valued for long-term safety assessment purposes because the model calibration is one of the key instruments (along with additional site investigations) for the uncertainty treatment, and accurate models are usually highly computationally expensive. Hence, the proposed method could become a noticeable contribution to the uncertainty management framework within safety assessment computational tools.

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