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Reply on RC2

Vanja Travaš et al.

Author comment on "Estimation of hydraulic conductivity functions in karst regions by particle swarm optimization with application to Lake Vrana, Croatia" by Vanja Travaš et al., Hydrol. Earth Syst. Sci. Discuss., https://doi.org/10.5194/hess-2022-253-AC3, 2023

REMARK: This manuscript estimated the hydraulic conductivity using particle swarm optimization method and analyzed the effect of protection method for the lake Vrana. The topic is somehow interesting, however, I have some major concerns for this manuscript as shown below:

ANSWER: We would like to thank the reviewer for all the remarks and comments, and we hope that with the answers given below and the changes made in the paper we managed to achieve the required quality for publication. We responded to all the comments and suggestions, and based on them, we believe that we have made appropriate corrections in the paper, which are marked with blue text. Please note that we have made corrections and adaptations in the paper based also on the remarks and suggestions of other reviewers and so some corrections can overlap.

REMARK: The introduction is not well organized. A literature review for the optimization method for the hydrological model and groundwater flow model is missing. Therefore, why do you select the particle swarm optimization method and not select other methods? I suggest to add an introduction for the literature review for the method of optimization of model parameters.

ANSWER: We have reorganized the introduction. In order to explain the issue of calibrating hydrological and groundwater models in more detail, we have further elaborated and enlarged the introduction and accordingly increased the list of literature (the last paragraph of the introduction has been completely replaced and significantly expanded). Apart that, in the introduction we also stated the problem of multimodality and used it as an argument for the application of the PSO method. Other organizational corrections were made in the introduction (all marked in the new version of the paper). A new part of the introduction (the last paragraph of the introduction), as well as the newly introduced references, are listed below.

\bibitem[Beasley et al. (2012)]{Beasley1993}

Beasley, D., Bull, D.R., and Martin, R.R.: A Sequential Niche Technique for Multimodal Function Optimization, Evolutionary Computation, 1(2), 101-125, doi: 10.1162/evco.1993.1.2.101., 1993.

\bibitem[Beven (2006)]{Beven2005}

Beven, K.J.: A manifesto for the equifinality thesis, J. Hydrol., 320(1-2), 18-36, 2006.

\bibitem[Charlier et al. (2012)]{Charlier2012}

Charlier, J.-B., Bertrand, C., and Mudry, J.: Conceptual hydrogeological model of flow and transport of dissolved organic carbon in a small Jura karst system, J. Hydrol., 460-461, 52-64, https://doi.org/10.1016/j.jhydrol.2012.06.043, 2012.

\bibitem[Haddad et al. (2013)]{Haddad2013}

Haddad, O.B., Tabari, M.M.R., Fallah-Mehdipour, E., and Marino, M.A.: Groundwater Model Calibration by Meta-Heuristic Algorithms, Water Resources Management, 27, doi:10.5281/zenodo.1287350, https://doi.org/10.1007/s11269-013-0300-9, 2013.

\bibitem[Lu et al. (2018)]{Lu2011}

Lu, C., Shu, L., Chen, X., and Cheng, C.: Parameter estimation for a karst aquifer with unknown thickness using the genetic algorithm method, Environ Earth Sci, 63, 797-807, https://doi.org/10.1007/s12665-010-0751-8, 2011.

\bibitem[Mahmoud et al. (2021)]{Mahmoud2021}

Mahmoud, E.A., Hossam, A.A., Kassem, S.E., and Mohsen, M.E.: Estimation of groundwater recharge using simulation-optimization model and cascade forward ANN at East Nile Delta aquifer, Egypt, Journal of Hydrology 34, doi:10.5281/zenodo.1287350, https://doi.org/10.1016/j.ejrh.2021.100784, 2021.

\bibitem[\"Ozcan and Yilmaz (2007)]{Ozcan2007}

\"Ozcan, E., and Yilmaz, M.: Particle Swarms for Multimodal Optimization, Adaptive and Natural Computing Algorithms, 4431, https://doi.org/10.1007/978-3-540-71618-141, 2007.

\bibitem[Rimmer and Salingar (2006)]{Rimmer2006}

Rimmer, A., and Salingar, Y.: Modelling precipitation-streamflow processes in karst basin: The case of the Jordan River sources, J. Hydrol. 331, 524-542, https://doi.org/10.1016/j.jhydrol.2006.06.003, 2006.

\bibitem[Wheater et al. (2022)]{Wheater1986}

Wheater, H.S., Bishop, K.H., and Beck, M.B.: The identification of conceptual hydrological models for surface water acidification, Hydrol. Processes, 1(1), 89-109, https://doi.org/10.1002/ hyp.3360010109, 1986.

\bibitem[Wunsch et al. (2022)]{Wunsch2022}

Wunsch, A., Liesch, T., Cinkus, G., Ravbar, N., Chen, Z., Mazzilli, N., Jourde, H., and Goldscheider, N.: Karst spring discharge modeling based on deep learning using spatially distributed input data, Hydrol. Earth Syst. Sci., 26, 2405-2430, https://doi.org/10.5194/hess-26-2405-2022, 2022.

\bibitem[Ye et al. (1997)]{Ye1997}

Ye, Ye, Bates, B.C., Viney, N.R., Sivapalan, M., and Jakeman, A.J.: Performance of conceptual rainfall-runoff models in low-yielding ephemeral catchments, Water Resour. Res., 33(1), 153-166, doi:10.1029/96WR02840, 1997.

\bibitem[Zambrano-Bigiarini and Rojas (2020)]{Zambrano2020}

Zambrano-Bigiarini, M., and Rojas, R.: hydroPSO: Particle Swarm Optimisation, with Focus on Environmental Models, R package version 0.5-1, doi:10.5281/zenodo.1287350, https://CRAN.R-project.org/package=hydroPSO, 2020.

Regardless of the adopted approach, the success of model calibration can be depended on the number of parameters that are subject of calibration. Namely, for a lumped karst model in which the exchange of water between interconnected karst region is modeled by more than one ODE, a different values of calibration parameters can result in similar model prediction \citep{Wheater1986,Ye1997}. In other words, there may be multiple solutions (known as multimodality) which consequently leads to unreliability in the physical interpretation of model parameters \citep{Beven2005}. In order to reduce the influence of overparameterization and obtain a unique solution, the number of all possible solutions should be reduced by introducing additional constraint conditions imposed on calibration parameters. If no generic property can be defined for a particular calibration parameter, by which the constraint condition can be formulated, the additional constraint conditions are obtained through analysis on the relative relationships between the available hydrological time series (which is often carried out by correlation and cross-correlation analyses). In other words, solving multimodal problems most often requires the application of an algorithm for pattern recognition in the available hydrological time series. For this reason, it should not be surprising that artificial neural networks \citep{Kurtulus2010,Hu2008,Coppola2003,Coulibaly2001} and different machine learning

methods \citep{Wunsch2022} have found their application in calibration of lumped karst models. However, the mentioned approaches are not that suitable in cases where the constraint conditions are known in advance and are given in the form of mathematical inequalities (as was the case in this paper). In such cases, it is opportune to treat the calibration of model parameters as an optimization problem \citep{Beasley1993} in which multimodality is commonly encountered. In such circumstances, the calibration of model parameters requires the definition of objective function that is depended on design variables (i.e. model parameters). Since the objective function is usually defined as a measure of difference between the considered predicted value and the one obtained by field measurements, the calibration of model parameters is reduced to its minimalization. For this purpose, the domain of the objective function is searched in an iterative fashion. Unless a specific search (local search) of the domain of the objective function is expected, the parameters of a karst model can be effectively calibrated by genetic algorithms \citep{Lu2011}. For more demanding optimization problems, in which it is expected that the objective function has many local minima permeated throughout the entire domain of the objective function (multimodality), both global and local search is necessary. In these situations, the bio-inspired algorithm known as particle swarm optimization (PSO method) is more suitable because it is based on simultaneous local and global search of the domain of the objective function \citep{Qian2019} and so, it is very attractive for solving multimodal problems \citep{Ozcan2007}. Moreover, this approach has previously been successfully applied to calibrate groundwater flow models in alluvial aquifers \citep{Haddad2013,Mahmoud2021} but also for calibrating flow parameters in environmental models \citep{Zambrano2020}. In order to examine the application of the PSO method and indicate the possibilities it offers in a contest of karst modeling, it was applied to the estimation of hydraulic conductivity functions used for modeling the exchange of fresh and salt water in lake Vrana, Croatia.

REMARK: The assumption of fully turbulent and partially saturated water flow through karst conduits is used and the Darcy's flow is neglected for the groundwater flow simulation. Does this assumption cause uncertainty for the simulation? The reasonability for this assumption need further explanation. The hydrogeology conditions for the study area need some more detail introduction.

ANSWER: The introduced assumption certainly causes uncertainty, but with negligible influence for the scope of the model. Namely, the assumption can be justified by the purpose of the model, which was to describe the mass exchange of salt and fresh water between the lake and the sea. For this purpose, it should be noted that the lake is located in the immediate vicinity of the sea and that even a relatively small pressure gradients are reflected in the rapid exchange of water through karst conduits (which was also determined by field measurements in cases of different sea and water levels in the lake). The Darcy's flow cannot compete in the rate of exchange of these quantities of water and is therefore justifiably neglected. In the same time, in the used framework of lumped karst models the Darcy flow component is not naturally included and combined modeling requires the application of the dual porosity model which cannot be linked to the subject of this paper which is devoted to the application of PSO methods for calibration of hydraulic conductivity functions. The hydrogeology conditions of the study area are further elaborated in the title Study area where the text below is added.

Within the basin of lake Vrana, few groups of rocks can be recognized \citep{Rubinic2014}. First of all, these are Upper Cretaceous limestones, i.e. very

permeable rocks within which an underground hydrographic network has been developed. On the other hand, it is also possible to determine the area within which the dolomites and limestones of the lower part of the Upper Cretaceous alternate, forming a medium permeable layer that can slow down the flow of underground water. Finally, a large part of the basin consists of impermeable or very poorly impermeable flysch deposits that in some places cause the formation of surface flows. For calibrating the model parameters, these surface flow components will be set based on known \textit{in situ} measurements. On the other hand, the groundwater flow components, which are realized as a consequence of the developed hydrographic network in the Upper Cretaceous limestones, will be modeled using the semi-distributed lumped karst model, relying on the assumption of a fully turbulent flow.

REMARK: For the parameter optimization, it is necessary to show the process for the seeking the optimal parameters, and how about the efficiency of this method? I suggest to add some comparison of this method and other traditional method.

ANSWER: To illustrate the convergence characteristics of the optimization procedure, a Figure has been added in the paper that shows the change in the global optimum during iterations (the best values of the objective function up to that iteration). It should be noted that complete convergence with a negligible error is not possible for the reason that the aforementioned would require a more detailed parameterization of the calibration functions (with more than 60 points – this comment is also important and is introduced in this new part of the paper). On the other hand, a more detailed parameterization of the calibration functions would make the calibration problem far more complex and would drastically affect the efficiency of the aforementioned method. Namely, in that case, the search space would be much larger, i.e. with a much larger number of dimensions. The efficiency of the method decreases drastically with the increase in the number of optimization variables, but at the same time it should be noted that it is subject to parallelization and that within one iteration the searching procedure of each particle is independent all other particles (which is attractive for openMP parallelization). Regarding the comparison of this method with other similar methods, it should be noted that for the given framework (lumped karst model) only automated calibration methods can compete (neural networks, deep search, genetic algorithms, etc.). On the other hand, although there are essential differences between the above, the PSO method is particularly attractive for the reason that it offers a simple implementation of constraints conditions over calibration parameters and for the reason that it performs global and local search simultaneously (which solves the problem of multimodality). For the description of the convergence, we have added the text attached below.

The convergence of the optimization process is illustrated in figure \ref{fig08} which shows the value of the objective function at points $\textbf{x}_{g,best}^{(e)}$ of the global optimum respect to the iteration number. For the adopted parametrization of the calibration functions, the objective function reached the lowest possible value, and further reduction of its value would require a larger number of parameters, i.e. a denser discretization of the calibration functions (more than 20 point per functions). On the other hand, such a procedure would significantly affect the number of necessary iterations to reach a smaller error, as well as the number of required particles (because the search space would be larger). In this sense, the parameterization of the calibration functions is determined based on a compromise between computational time and acceptable minimum value of the objective function.

REMARK: A discussion for the comparison of results and method of this study and other similar studies are need.

ANSWER: For these purposes, we have added the text below.

In order to compare the presented approach with other approaches, it should be emphasized that the framework of the model is defined by a system of two ordinary and non-linear differential equations with variable coefficients that also define the calibration functions. In these circumstances, automated methods such as genetic algorithms are usually used \citep{Lu2011,Nematolahi2018}. On the other hand, if by the method of trial and error it is determined that the model results are significantly sensitive to the calibration functions (model parameters), the application of genetic algorithms is probably not the most appropriate. Namely, this sensitivity of model results to calibration functions indicates a large number of local minima of the objective function by which the multimodality of the problem can be recognized. In such circumstances, it is not only necessary to carry out a global search of the domain of the objective function, as carried out by the method of genetic algorithms, but it is also necessary to examine local minima, that is, to enable a more detailed search of individual parts of the domain by carrying out local searches. Moreover, the search for local minima must be adaptive so that the solution in the current iteration can be updated by the new local solution that results in a more favorable variant of the calibration parameters. In this way, the possibility of searching for a larger number of local minima is realized, which is necessary for such multimodal problems. Considering all of the mentioned, and by noting that the model in question showed the characteristics of multimodal problems, the calibration of the model was performed using the PSO method which simultaneously performs global and local search of the domain of the objective function \citep{Ozcan2007,Kuok2012,Zambrano2013}. Considering the experience gained from the performed analysis, the application of the PSO method can be recommended for the calibration of a semi-distributed lumped karst models based on a system of nonlinear ODEs.

REMARK: The conclusion seems too long, you can reduce some statements.

ANSWER: The conclusion is shortened.

Please also note the supplement to this comment:
https://hess.copernicus.org/preprints/hess-2022-253/hess-2022-253-AC3-supplement.pdf