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Using multi-objective optimisation to integrate alpine regions in groundwater flow models

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Abstract. Within the research project GLOWA Danube, a groundwater flow model was developed for the Upper Danube basin. This paper reports on a preliminary study to include the alpine part of the catchment in the model. A conceptual model structure was implemented and tested using multi-objective optimisation analysis. The performance of the model and the identifiability of the parameters were studied. A possible over-parameterisation of the model was also tested using principal component analysis.

1 Introduction

Within the framework of the GLOWA-Danube project (Mauser and Barthel, 2004), a groundwater flow model was developed for the Upper Danube basin. The model is coupled to a soil water balance model and a hydraulic surface water model. From the former it receives the infiltration rate through the lower boundary, defined at two meters below the land surface at every grid cell. To the latter it delivers a water exchange rate between the aquifers and the surface waters for every river cell. Wolf et al. (2004) reported in detail on the chosen hydrogeological conceptual model, on the difficulties encountered during the work on the numerical flow model (MODFLOW, McDonald and Harbaugh, 1988) and on the solutions found for these difficulties. The presence of the alpine region in the south of the Upper Danube basin posed a consistency problem between the groundwater and the soil models. Due to their steep, folded and faulted internal structure, the Alps, with the exception of the alluvial aquifers in valleys, are not compatible with the Darcy-Law based MODFLOW approach. A solution had to be found to fill the gap between the two models in the alpine part of the catchment.

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2 Modelling structure

The task is to develop a model for the subsurface flow in the alpine regions which should link the soil water model, concerned with the first two meters of soil and the groundwater model dealing with the flow in the alluvial valley aquifers. The absence of deterministic information regarding the fractures dominated subsurface flow beneath the mountain slopes obliges the use of a conceptual hydrological approach based on a qualitative description of the involved processes.

The proposed modelling structure is presented in Fig. 1. Based on the existing river gauges, alpine subcatchments have been delineated. For every subcatchment the infiltration computed by the soil water model is split into two parts: the infiltration above alluvial valleys and above mountains slopes. First, the infiltration above the alluvial valleys aquifers is injected as vertical groundwater recharge into the MODFLOW model. Second, the infiltration above the mountainous slopes is aggregated over the subcatchment and again separated in two parts. The first part, named *interflow* in the context of this paper, exfiltrates along the slope to flow directly into the river network. The second part flows through the mountain to exfiltrate in the alluvial aquifer as lateral groundwater recharge. The water exfiltrating from the valley aquifer into the rivers is named here *baseflow*. For the water routing through the individual components, conceptual modelling units were used based on the linear storage cascade concept (Nash, 1959). Each of the storage cascades is defined by two parameters, namely the number of reservoirs n and the reservoir coefficient k. The parameter s, determining the separation between interflow and baseflow, and the parameters of the storage cascades units n_i, k_i are being quantified during the calibration process because no direct physically-based information is available for that purpose.

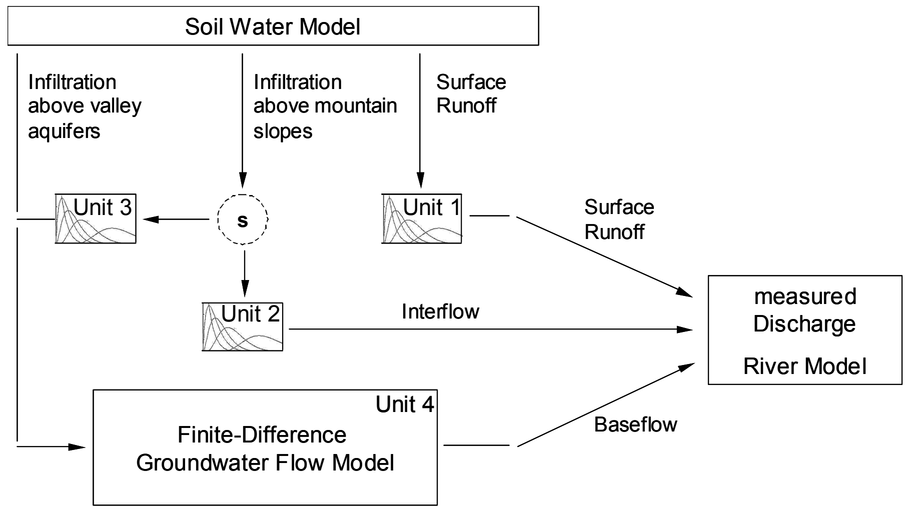

Fig. 1. Structure of the proposed conceptual model integrating the Alps in the groundwater model.

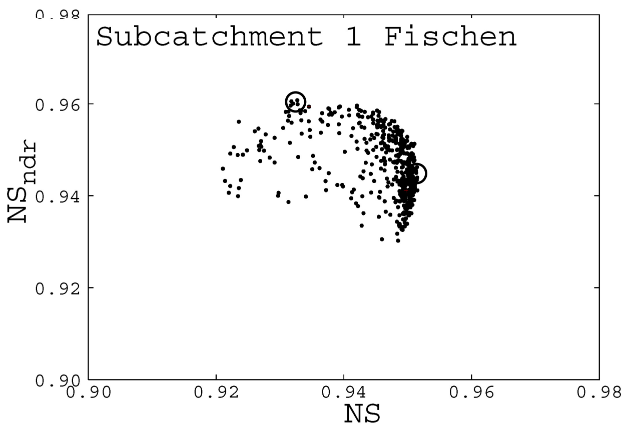

Fig. 2. The Pareto set represented in the space of two objective functions. The Pareto front is orientated towards the upper right corner, which represents the perfect fit. The circles mark the single-objective optima.

The task to be solved now is to determine physically-interpretable sensitive parameters (relative to the available data) for the model structure presented in Fig. 2. In a preliminary approach presented here, the MODFLOW model was also replaced with a linear storage cascade. The proposed testing procedure for the model structure requires a large number of model evaluations and would not be applicable with the MODFLOW model due to the needed CPU time.

3 Methodology

The developments in the last decade in the field of hydrological modelling have made clear that good fits between measured and simulated discharge curves, evaluated using one performance criteria, are by far not enough to consider a problem solved. Even when using state-of-the-art automatic calibration algorithms one cannot avoid the problems generated by the numerous local optima with very similar performance criteria values (see Duan et al., 1993), by the subjectivity involved in the selection of this criterion and by the "equifinality" issue (the existence of many parameter sets leading to almost equally good model results, see Beven, 2000). There are several possible answers to these problems, which do not oppose, but rather complement each other. One answer is a generalised sensitivity analysis (Hornberger and Spear, 1981) or the GLUE approach derived from it (Beven and Binley, 1992).

Another answer, the one applied here, is the use of a multi-objective calibration as opposed to a simple one objective calibration (see Gupta et al., 2003). No objective function characterises in an exhaustive manner the quality of the fit between the measured ($\boldsymbol{Q_{mes}}$) and the computed ($\boldsymbol{Q_{sim}}$) time series. For a long time, this was the main argument in favour of the manual calibration. Although less systematic, less reproducible and much more time consuming, the manual calibration had the advantage of being able to lead to an optimum which takes more than one mathematical expression for the quality of the fit into consideration. This weakness was solved for the automatic approach by the use of multi-objective calibration procedures. The result of the calibration is in this case no longer one single parameter set, but a group of parameter sets, termed Pareto sets, which optimise as a group several predefined objective functions. Having a range of optimal parameter sets and optimal model results offers an additional advantage. Through the analysis of the spread of these ranges, one can quantify in a more objective manner the degree of confidence that one should have in the given model. The dangerous feeling of certainty, which the modeller has when dealing with one optimal parameter set as a final answer of the problem, is thus at least partially eliminated.

Table 1. Optimal values for the five criteria used in the multi-objective analysis. All five criteria take values in the interval $(-\infty{:}1]$, with 1 indicating a perfect fit. The seven subcatchments were sorted according to the quality of the results.

	Calibration values					Validation values				
	NS	NS_{dr}	NS_{ndr}	SAE	NS_{tr}	NS	NS_{dr}	NS_{ndr}	SAE	NS_{tr}
Subcatch 1	0.952	0.893	0.961	0.941	0.977	0.978	0.967	0.980	0.938	0.980
Subcatch 2	0.950	0.920	0.920	0.931	0.957	0.965	0.947	0.957	0.923	0.967
Subcatch 6	0.945	0.939	0.926	0.885	0.930	0.937	0.925	0.926	0.868	0.927
Subcatch 3	0.916	0.888	0.830	0.853	0.889	0.905	0.863	0.895	0.855	0.889
Subcatch 4	0.757	0.767	0.615	0.731	0.689	0.615	0.502	0.588	0.728	0.671
Subcatch 5	0.568	0.565	0.318	0.605	0.516	0.486	0.431	0.484	0.588	0.491
Subcatch 7	0.406	0.231	0.189	0.465	0.373	0.285	0.032	0.224	0.404	0.279

For the case presented in this paper five objective functions were selected for a multi-objective analysis (see Freer et al, 2003): the Nash-Sutcliffe efficiency (NS), Nash-Sutcliffe efficiencies computed for the increasing and the decreasing part of the hydrographs (NS_{dr}, NS_{ndr}), $SAE{=}1{-}S$, where S is the sum of the absolute differences between $\boldsymbol{Q_{mes}}$ and $\boldsymbol{Q_{sim}}$ normalised by the sum of $\boldsymbol{Q_{mes}}$, and the Nash-Sutcliffe efficiency computed between $\boldsymbol{Q_{mes}}$ and $\boldsymbol{Q_{sim}}$ after applying a Box-Cox transformation (NS_{tr}). The five functions were computed for four time scales (one, two, seven and thirty days) and the average of the four values was used in the optimisation procedure. The computed Pareto sets were composed of 495 parameter sets, respecting the recommendation given by Gupta et al. (2003) of having around 500 values.

4 Test area: the Ammer catchment

The Ammer catchment, (709 m^2), located in the southwestern corner of Bavaria upstream of the Ammer lake, was chosen as a test area. Apart from the representativeness of the catchment for the transition zone between the alpine formations and the molasse zone, the choice was also motivated by the very good data availability. Seven subcatchments could be defined based on the existing river gauges. The analysed time period was 01.11.1990–01.01.2000. The last seven years of the time series were used for the calibration, the first three years were used for the validation. The necessary input data, the infiltration rate and the surface runoff, were calculated using the PROMET soil water balance model (Mauser, 1989) and were made available to the authors of this paper by Dr. Ralf Ludwig from the Ludwig Maximilian University in Munich.

5 Results and discussion

The multi-objective analysis was applied on the seven subcatchments of the Ammer catchment. Figure 2 shows the Pareto solution in the criteria space for one pair of objective functions. The Pareto front is clearly defined as well as the position of the single – objective optimums at the edge of the Pareto front. It is an indication that the objective functions were chosen correctly. Other performance criteria were tested before selecting the five functions previously mentioned. The root mean square error and the heteroscedastic maximum likelihood estimator proposed by various authors correlated to the Nash-Sutcliffe efficiency for this study case, so that the Pareto set was concentrated on the $y{=}x$ line, thus adding no additional information to the analysis.

The optimal values for the five performance criteria, averaged over the four time scales already mentioned, are presented in Table 1 for both the calibration and validation periods. For four of seven subcatchments the results can be qualified as very good, with all performance criteria having values between 0.85 and 0.98. The other three subcatchments make a distinct picture, two of them (4 – gauge Oberammergau and 5 – gauge Unternogg) having average results and the third (7 – gauge Obernach) being at the limit between poor and unacceptable.

Figure 3, presenting the measured versus the computed time series for the subcatchments with the best (1) and the worst (7) results, is helpful for explaining the poor results for the subcatchments 4, 5 and 7. By comparing the direct results of the soil water model – the sum between the infiltration rate and the surface runoff – with the measured river discharges, it is noticeable that the soil water model already has attenuated the initial rain signal too much. As the transport model here discussed can only transport the input signal forwards and increase its attenuation, there is no space for it to improve the results of the soil water model, which in this particular case would require a backwards transformation and a de-attenuation. It is interesting to notice that the three subcatchments, whose results are not satisfactory, are situated furthest upstream and are characterised by large altitude differences. The proper parameterisation of the soil layer is an extremely difficult process when it comes to very steep mountain slopes. The interpolated rain time series are also affected by a significant degree of uncertainty, although the correlation between rain and elevation was taken into consideration during the interpolation process (Ludwig, 2000).

For subcatchment 1, Fig. 3 confirms in a graphical form the very good fit between the measured and the computed time series. There is a slight tendency to underestimate the highest peaks, but otherwise the computed Pareto solutions

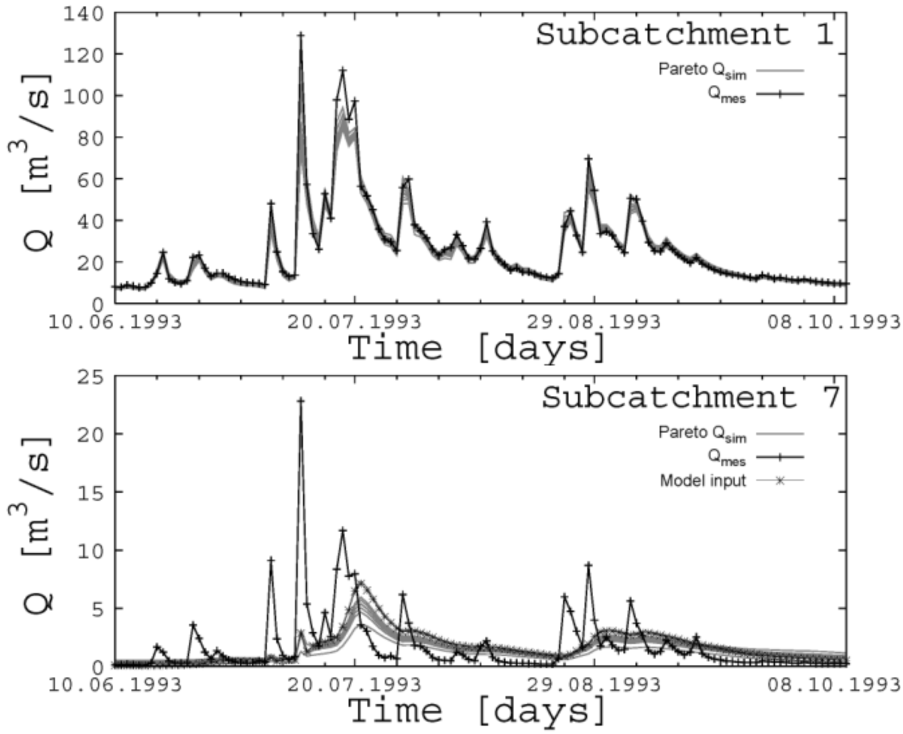

Fig. 3. Computed versus measured time series for the subcatchment with the best (1) and the worst (7) results. To explain the poor results in subcatchment 7 the model input (the results of the soil water model) was also represented.

are able to reproduce the dynamics of the measured discharge curve well. Notice should be also given to the thin range of values characterising the Pareto solutions. Although the Nash-Sutcliffe efficiency for this subcatchment is 0.95, the measured discharge is located inside the interval defined by the Pareto set in only 53% of the days from the calibration period and 48% of the days from the validation period. One goal of the multi-objective analysis, namely to create a solution set fully "including" the measured points (Gupta, 2003), could thus not be achieved. This result was also noticed during other studies and was used to criticise the over-interpretation of the Pareto set as a measure of the uncertainty of a model (Freer et al., 2003).

In addition to testing model performance, it is important to test whether the calibrated parameters are more than the results of a mathematical optimisation and can be interpreted in a physical way. Figure 4a shows the distribution of the 495 normalised Pareto solutions for the eleven model parameters for subcatchment 1. During the calibration, the parameters were restricted to positive values. The upper bound was imposed by restricting the two coefficients for every storage cascade unit and also their product (which is the time distance with which the centre of gravity of the input signal is translated into the output signal) to values predetermined on the basis of hydrograph separation methods (Schwarze et al., 1991).

The normalised values of the Pareto parameters in Fig. 4a show no trend, as it seems that combinations of values throughout the whole allowed spectrum were obtained after the optimisation process. The storage cascades' coefficients are agglomerated into the lower range only due to the forced restriction for every $n_i * k_i$ product to an upper bound. One possible explanation of the poor identifiability of the results is the over-parameterisation of the model and the parameter interdependence that comes with it. To test this hypothesis, the correlation matrix inside the Pareto set was computed and its eigenvalues and eigenvectors determined (principal component analysis, see Bishop, 1995). The analysis lead to relatively high correlation coefficients and to few dominant eigenvalues, strongly suggesting that the parameters are compensating each other in the optimisation process. Figure 4b shows the Pareto set tranformed into the eigenvectors. Although a certain degree of variability remains, the values are clearly defined, proving the over-parameterisation hypothesis. It is also worth mentioning that this analysis "catches" the linear interdependences only, which means that the computed number of needed independent parameters (the number of dominant eigenvalues) is certainly overestimated. Additional studies are needed to determine the non-linear dimensionality of the system.

6 Conclusions

For the integration of the alpine part of the catchment into a regional groundwater flow model, a conceptual model structure was tested using a multi-objective optimisation analysis.

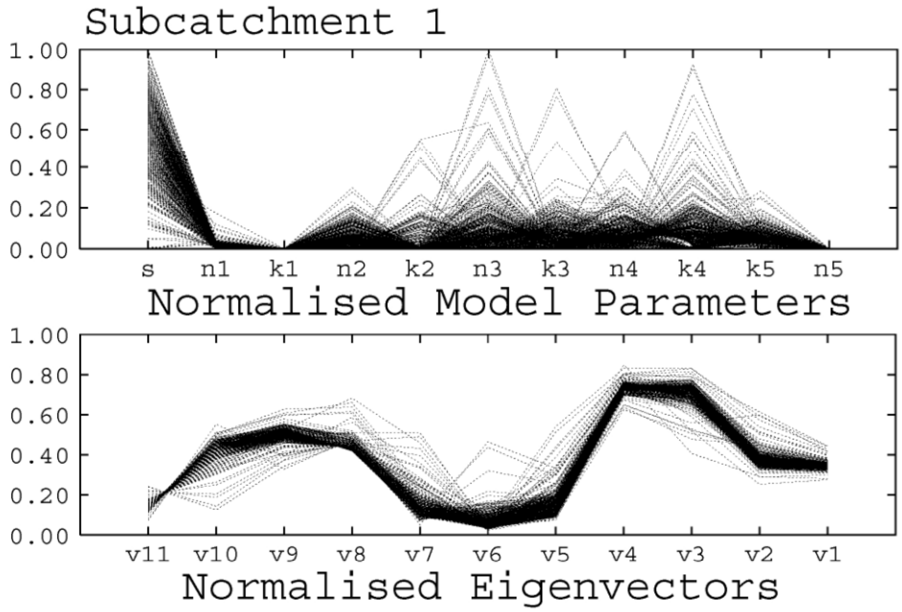

Fig. 4. (a) Normalised values of the Pareto set's parameters; **(b)** Normalised values of the Pareto set's eigenvectors. ***v*11** is the eigenvector explaining the smallest amount of parameter variability, ***v*1** the largest.

For most of the subcatchments of the test area, a good performance was achieved. The optimised parameters were poorly defined, and a clear over-parameterisation was identified which lead to strong correlations and compensation in the parameter space. Further studies are planed to test whether the inclusion of the groundwater model resolves this issue or whether a rethinking of the structure is needed.

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