Improved calibration of hydrological models: use of a multiobjective evolutionary algorithm for parameter and model structure uncertainty estimation¹

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1. Introduction

Powerful optimisation algorithms have become widely used for the automatic calibration of model parameters, and especially evolution-based methods have been found to be efficient in identifying the globally best parameter set. Current research in the area of automatic calibration also addresses the problem of using multiple criteria for the model optimisation, these criteria being calculated on one or different model outputs (see for example (Seibert, 2000), (Vrugt, et al., 2003)). An efficient global optimisation algorithm can reliably find the global optimal parameter set but the meaning of such a unique parameter set is questionable especially if its performance in terms of the optimisation objective is not significantly different from other solutions. This parameter uncertainty problem is addressed by recent studies through the application of Markov Chain Monte Carlo methods that become increasingly popular for the estimation of the posterior probability distribution of parameters (see for example (Kuczera and Parent, 1998), (Vrugt, et al., 2003)).

These different approaches are all based on a predetermined and fixed hydrological model structure. This structure is usually defined by the parameterisation of the phenomena the modeller judges significant to simulate the system behaviour. The design options have an important impact on the model's ability to reproduce the signal used for calibration and different model structures can lead to virtually the same calibration and validation results. The reproduction of some internal processes can sometimes help to identify the best model structure, the final choice depending essentially on the modeller's experience. If the calibrated model is applied to current climatic and hydrologic conditions, one might not be concerned about this problem. But for future conditions, especially in the context of climate change, the different model structures can lead to significantly different simulation results and the induced modelling uncertainty is potentially higher than the one due to the model parameter estimation uncertainty. An overall modelling uncertainty assessment should therefore not only be based on one fixed model structure but should include other equivalent model structures.

The present paper addresses the problem of identifying such apparently equivalent model structures by the application of a new clustering evolutionary multi-objective optimisation algorithm that has recently been developed for industrial design problems at the Laboratory of Industrial Energy Systems (Laboratorie d'Energie Industrielle - LENI) of the Swiss Institute of Technology in Lausanne. Using this algorithm, decision variables referring to the model design can be included in the parameter optimisation process and several equivalent model structures can be identified. Its application is illustrated through the joint parameter and model design optimisation for a reservoir based hydrological model that has been developed for climate change impact studies in a glacierized alpine catchment. Based on a case study in

¹ Schaefli, B., Hingray, B. and Musy, A., 2004. Improved calibration of hydrological models: use of a multi-objective evolutionary algorithm for parameter and model structure uncertainty estimation. In: B. Webb (Editor), Hydrology: Science and Practice for the 21st Century. British Hydrological Society, London, pp. 362-371.

the Swiss Alps, the model behaviour under the different optimal design options is illustrated for modified climatic conditions and the implications of model design optimisation are discussed based on these results.

2. The hydrological model

The hydrological discharge simulation is carried out at a daily time step through a conceptual, semi-lumped model developed by the authors. The model has two levels of discretisation. The ice-covered part of the catchment is first separated from the not ice-covered part. Next, both parts are subdivided into elevation bands. Each of the resulting spatial units is characterized by its surface and its hypsometric curve and is assumed to have a homogenous hydrological behaviour. The precipitation – runoff transformation is simulated for each spatial unit separately; the runoff contributions of all units are added to provide the total discharge at the outlet of the entire catchment. Figure 1 shows the basic hydrological model structure for a given spatial unit, the different submodels and their interconnections. Hereafter, the basic design of each submodel and the possible variants are presented.

In the model structure presented, the glacier surface is supposed to be constant for a given simulation period. For the future scenario simulation, the ice-covered surface has to be updated. In the present study, this update is based on the assumption that the mean interannual accumulation area ratio (AAR) (Anonymous, 1969) simulated for observed climatic conditions remains constant in the future. For a given hydrological year (starting on the 1st October), the AAR is computed from the sum of spatial units that experience snow accumulation.

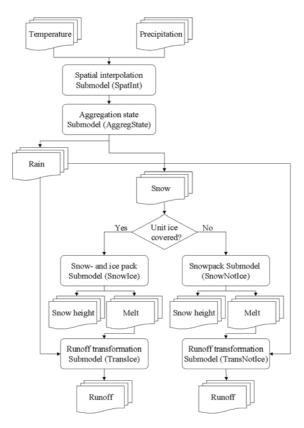


Figure 1: Basic hydrological model structure (for one spatial unit) showing the different submodels and the input and output time series; in brackets: the submodel short names

Spatial interpolation submodel

The temperature and precipitation time series are linearly interpolated according to the mean elevation of the spatial unit. The temperature decrease with altitude is fixed to 0.65 °C per 100 m of altitude change

(the mean gradient of observed temperature series in the Swiss Alps). The precipitation increase factor $(c_{precip} [\%/100m])$ is included in the parameter optimisation procedure as little knowledge about the local altitudinal variation of the precipitation can be derived from observed data.

Aggregation state submodel

The aggregation state submodel computes the nature of precipitation (liquid or solid) and is based on a fuzzy rule (Equation 1):

$$P_{snow} = \max\{0, \min\{P_{tot}, P_{tot}(T_{50} + T_{Trans} - T)/(2T_{Trans})\}\}$$

$$P_{liq} = P_{tot} - P_{snow}$$
(1)

where P_{snow} [mm d⁻¹] is the snowfall, P_{tot} [mm d⁻¹] the total precipitation, P_{liq} [mm d⁻¹] the rainfall, T [°C] the air temperature, T_{50} [°C] the temperature that corresponds to 50 % of the precipitation falling as snow and $2T_{Trans}$ [°C] the length of the temperature interval over which snowfall and rainfall occurs simultaneously.

Snow pack submodel (not ice-covered spatial units)

The snow height is computed as the difference of incoming snowfall and outgoing snowmelt, M_{snow} [mm d⁻¹] that is computed according to a classical temperature-index approach (Equation 2).

$$M_{snow} = \begin{cases} a_{snow}(T - T_m) & T > T_m \\ 0 & T < T_m \end{cases}$$
 (2)

where a_{snow} [mm d⁻¹ °C⁻¹] is the degree-day factor for snowmelt, T [°C] the mean temperature and T_m [°C] the threshold temperature for melting that is set to 0°C. In the basic model configuration, the water flow from the snow pack corresponds to M_{snow} . We also include a more complex approach in the optimisation procedure based on (Kuchment and Gelfan, 1996). This approach assumes that the snow pack has a capacity of retention θ_{snow} and that water flow only occurs if this capacity is reached.

Snow and ice pack submodel (ice-covered spatial units)

On the ice-covered spatial units, the water is stored in three different forms, as snow, ice or firn, the last form being the transition state between snow and ice. The evolution of the snow pack is simulated as in the snow pack submodel. At the end of each hydrological year (30th September), the snow that has fallen during the year but not melted is added to the firn pack. The evolution of this compartment is simulated with the same approach as for snow (Equation 2), using a degree-day factor for firn, a_{firn} [mm d⁻¹ °C⁻¹], but melt only occurs if the snow pack has disappeared. If at a given day, a spatial unit is covered neither by snow nor by firn, the underlying ice melts according to Equation 2 with a degree-day factor a_{ice} [mm d⁻¹ °C⁻¹]. For the optimisation procedure, we also consider a model variant that uses only snow and ice, i.e. no transition between the two forms occurs.

Runoff transformation submodel for ice-covered units

The rainfall and melt transformation into runoff is based on the model of (Baker, et al., 1982), who use three parallel linear reservoirs to simulate the water transport to the outlet, one reservoir each for snow, firn and ice. The basic linear reservoir approach is given in Equation 3.

$$Q_{j}(t) = Q_{j}(t-1) e^{-\frac{1}{k_{j}}} + I_{j}(t) (1 - e^{-\frac{1}{k_{j}}})$$
(3)

where $Q_j(t)$ [mm d⁻¹] is the discharge from the reservoir j (j = snow, firn, ice) at time step t and $Q_j(t-1)$ the discharge at the previous time step. k_j [d] is the storage constant of the reservoir j and $I_j(t)$ [mm d⁻¹] is water inflow into the reservoir j that corresponds to the sum of melt water and rainfall.

Runoff transformation submodel for not ice-covered units

The rainfall – runoff transformation is carried out through a conceptual reservoir-based model named SOCONT developed in our research group and similar to the GR-models (Edijatno and Michel, 1989). It is composed by two reservoirs, a linear reservoir for the *slow* contribution and a non-linear reservoir for direct or *quick* runoff. Figure 2 shows the model in detail.

In the basic model form, the snowmelt – runoff transformation is simulated based on Equation 3 with j = snow. The following model variant is used for the optimisation procedure: rainfall and snowmelt are summed to an *equivalent rainfall* that is transformed into runoff through the model SOCONT.

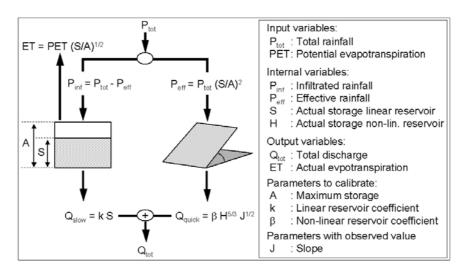


Figure 2: Rainfall-runoff transformation model SOCONT for not ice-covered spatial units

3. Optimisation algorithm

The optimisation tool used in the present study is the so-called Queueing Multi-Objective Optimiser (QMOO) that has been developed at LENI and is presented in detail in (Leyland, 2002). This algorithm has been developed in order to improve the optimisation performance on problems of energy system design but is applicable to a wide range of optimisation problems. It has been tested successfully on several theoretical test problems and has been proven to be robust and effective for the resolution of non-linear, non-continuous and mixed real – integer problems in the domain of optimisation of energy systems ((Leyland, 2002), (Burer, et al., 2003)) The test problems as well as the real world problems showed that QMOO successfully optimises most of them without requiring any specific tuning to each problem (Leyland, 2002). This means that the algorithm is particularly useful for non-specialist users. In the domain of hydrological model calibration, most recent optimisation tools still require tuning (see for example (Reed, et al., 2003), (Vrugt, et al., 2003)) and consequently, the user needs to acquire experience in the application of the algorithm or should have a good idea about the behaviour of the problem to optimise.

QMOO is a new generation clustering evolutionary algorithm that handles integer problems (i.e. problems including decision variables of integer type). The algorithm is multi-objective, i.e. it identifies the Pareto-optimal solutions for multiple objective functions. The Pareto-optimality (Pareto, 1896) can be interpreted as follows: a point of the decision variable space is Pareto-optimal if no other point is better in all objectives. The set of all Pareto-optimal points is called Pareto-optimal frontier. Rather than just identifying the global Pareto-optimal frontier, QMOO finds and retains many local Pareto-optimal frontiers - a property that allows the identification of multiple solutions. It is obtained through cluster analysis techniques that ensure local competition between sets of decision variables (so-called *individuals*) in the decision variable space and that allow the identification of separate local optima simultaneously. This property preserves diversity and helps the algorithm to converge to difficult-to-find optima. In the

following, the key features of the algorithm – from the point of view of the application presented in this paper - are briefly reviewed.

Most multi-objective evolutionary algorithms are generation based (in the area of hydrological modelling see for example (Seibert, 2000), (Reed, et al., 2003)), i.e. all individuals are replaced at the same time. QMOO on the other hand is *steady-state* – creation and removal of an individual are completely separate processes. The current population always contains the – in a Pareto sense - best individuals found so far – or at least as many of them as is practical to store. The algorithm is therefore extremely elitist. The diversity is preserved by dividing the individuals into groups using clustering methods from statistical analysis. The careful choice of the individuals to be removed ensures that convergence continues throughout the optimisation. According to (Leyland, 2002), another unique property of QMOO is its approach to choosing the combination and mutation operators that are used to assign parameter values to an individual. These operators are chosen according to an evolutionary process including stochastic operator choice. The user of the algorithm therefore does not have to choose the appropriate operators for a given problem.

When applying QMOO to an optimisation problem the user must define a priori the number of clusters that are expected to be found. Even if certain clustering techniques can theoretically find the correct number of clusters contained in a data set, none of the techniques tested by (Leyland, 2002) could find the number of clusters in practice. However, this maximum cluster number should not be considered as a tuning parameter of the algorithm: it does not influence the quality of the global optimal solution found by the algorithm but the quantity of additional information provided by a single optimisation run. The number of clusters therefore reflects the diversity of solutions the modeller would like to obtain. In the present optimisation problem, the set-up of the maximum cluster number is straightforward: we would like to optimise all model structures simultaneously and we therefore set the cluster number equal to the number of different model structures. This maximum cluster number is not necessarily achieved as the optimisation algorithm sometimes finds fewer clusters than asked by the modeller.

4. Optimisation procedure

Decision variables

The hydrological model to optimise has up to 14 parameters or decision variables to calibrate (the exact number is depending on the model structure). Additionally, we integrate in the optimisation procedure 3 decision variables that refer to the model structure and that are of integer type. Each of the values that can be assigned to them corresponds to a specific submodel set-up. Table 1 presents all the decision variables, their lower and upper boundaries and their meaning. The possible value ranges retained for the model parameters are considerably enlarged compared to values that can be found in literature.

Optimisation objectives

The presented hydrological model has two different outputs that can be used for model calibration: i) the daily discharge at the outlet of the catchment and ii) the variation in space and time of the snow and ice pack for each elevation band. This last output enables the model to simulate the mass balance of the ice-covered units as the difference of incoming snowfall and outgoing melt water over a given period. The overall mass balance of the ice-covered part of the catchment can therefore be estimated for each year according to the method presented by (Aellen and Funk, 1990). The resulting series of simulated annual mass balances can then be compared to observed values obtained by direct glaciological measurement methods. In high mountainous catchments, the glaciers represent the most important water storage reservoir. The glacier mass balance estimated over long time periods is thus a good integrator of the overall water balance of the catchment.

For the present case study we use only two different objectives – this facilitates the interpretation of the results - even if at LENI QMOO has been tested successfully with more objectives. The first objective is based on the classical Nash criterion (Nash and Sutcliffe, 1970) calculated on the observed and simulated

river discharge series. In order to minimise the objective function, we use the Nash criterion complement to 1. The second objective is the absolute bias between the observed and simulated annual glacier mass balance. In the present context, the bias - even though it is known not to be very discriminative - is a necessary condition for judging the quality of a simulation. The exclusive use of objective functions based on quadratic error could lead to a biased discharge and mass balance estimation.

Table 1: Possible value ranges for the decision variables and the corresponding submodels (for abbreviations see Figure 1)

Variables	Min.	Max.	Type	Submodel	Meaning
V_{Ice}	2	3	Integer	SnowIce	Number of snow / ice types
V_{Melt}	0	1	Integer	SnowIce, SnowNotIce	0: Basic model, 1: With retention capacity
V_{Runoff}	0	1	Integer	TransNotIce	0: Basic model, 1: Equivalent rainfall in SOCONT
c_{precip}	-25	25	Real	SpatInt	Precipitation increase factor
T_{50}	-10	10	Real	AggregState	Central value of interval
$T_{Trans} \\$	0	10	Real	AggregState	Temperature Interval width
a_{gl}, a_f, a_n	0.1	25	Real	SnowIce, SnowNotice	Degree-day factors for ice, snow, firn
θ_f,θ_n	0	1	Real	TransIce, TransNotIce	Retention capacities for firn, snow
k_{gl}, k_f, k_n	0.01	90	Real	TransIce, TransNotIce	Storage coefficients for ice, snow, firn
log(k)	-16	-0.1	Real	TransNotIce	Slow reservoir coefficient
A	1	10000	Real	TransNotIce	Max. storage of slow reservoir
β	1	60000	Real	TransNotIce	Quick reservoir coefficient

5. Case study

In the present study, the hydrological model has been applied to a catchment situated in the Southern Swiss Alps, the catchment of the Rhone river measured at Gletsch (see Figure 3a). Table 2 gives some important physiographic characteristics of the catchment. The estimated mean annual precipitation at the mean altitude of the catchment is about 2550 mm and the mean daily temperature -5.0°C (reference period 1981-1999).

Table 2: Main physiographic characteristics of the case study catchment

Characteristic V	⁷ alue
Area [km ²] 3	88.9
Glaciation [%] 5	52.2
Mean slope [°]	22.9
Min. altitude [m a.s.l.]	755
Mean altitude [m a.s.l.]	2713
Max. altitude [m a.s.l.]	8612

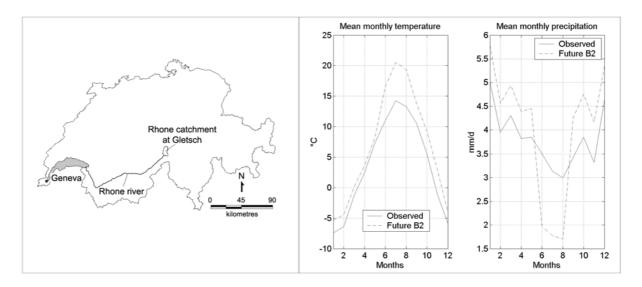


Figure 3: a) Location of the case study catchment in the Swiss Alps © Swiss Federal Office of Topography, b) interannual mean monthly precipitation and temperature for observed period (1983–1987) and future climate scenario B2 (2093 – 2097)

Data collection

The model needs three input time series, namely daily mean values of temperature, precipitation and potential evapotranspiration. We use precipitation and temperature time series from a meteorological station located within a few kilometres distance of the catchment. The potential evapotranspiration (PET) time series is calculated based on the Penman-Monteith version given by (Burman and Pochop, 1994). The daily mean discharge is measured at the outlet of the catchment. We used the period 1978 to 1982 for calibration and 1983-1987 for validation. For bi-objective optimisation, we used the observed annual mass balance of the Rhone glacier given for the hydrological years 1979/80 to 1981/82 by (Funk, 1985). As an illustration for future climate conditions, we used the method presented by (Shabalova, et al., 2003) to perturb the observed temperature and precipitation series based on a regional climate model output provided by the Hadley Centre for Climate Prediction and Research. The regional model is the HadRM3H model and the perturbation of observed time series is carried out according to the difference between the control run for the period 1960 – 1989 and the future scenario run for 2070 – 2099 that is based on the IPCC scenario B2 (Houghton, 2001). Figure 3b illustrates the observed time series and the corresponding climate change scenario. The scenario PET is interpolated as a function of the scenario temperature.

6. Results

Model optimisation for present climate

The algorithm is applied using an initial population of 500 individuals and setting the number of clusters to 8 that corresponds to the number of possible model set-ups. QMOO identifies only 4 clusters for the given objectives, each of the clusters corresponding to a different model set-up. The algorithm converges quickly, after 9000 model evaluations the local Pareto-optimal frontiers are identified. They are shown in Figure 4a. The algorithm is specially designed to preserve the tail ends of the Pareto-frontiers. This feature explains the "outliers" of cluster 3 and 4 (see Figure 4a). Note that the point density of these frontiers depends on the ability of the algorithm to handle large populations that is essentially limited by computational resources. In the present application, a Matlab® version of QMOO is used on a personal computer, which limits the handled population size to around 80 individuals, about half of them being locally non-dominated when the algorithm stops after a fixed number of objective evaluations.

The found solutions have Nash-values between 0.90 and 0.94 and a bias between 0 and 0.26. This apparently little trade-off has to be interpreted in the presented simulation context. For highly glacierized

catchments, high Nash-values are easy to achieve as long as the model reproduces the strong seasonality of the discharge. If we use a very simple model corresponding just to the mean observed discharge for each calendar day, we obtain for the Rhone catchment a Nash value of 0.85 and a bias of 0.02. Consequently there is an important trade-off between solutions having a low bias but Nash-values of 0.9 and solutions having a Nash-value around 0.94 but a bias of 0.26.

Table 3 summarises the mean optimal values of the decision variables for each solution cluster.

Table 3: Mean values of the decision variables for each solution cluster

Decision variable	Cluster 1	Cluster 2	Cluster 3	Cluster 4
V_{Ice}	2	3	3	2
V_{Melt}	0	0	1	1
V_{Runoff}	0	1	1	0
C _{precip}	3.1	18.6	7.8	3.4
T_{50}	3.2	3.4	-3.2	1.9
T_{Trans}	2.5	5.5	4.8	2.7
$a_{ m gl}$	10.8	16.8	9.7	10.4
a_{f}	-	12.9	14.6	-
a_n	10.1	3.9	8.7	9.9
$ heta_{ m f}$	-	-	0.34	-
Θ_{n}	-	-	0.23	0.55
k_{gl}	2.7	42.9	2.8	3.3
$k_{\rm f}$	-	16.3	23.3	-
k_n	28.5	8.3	21.5	27.2
log(k)	-8.8	-7.4	-10.1	-9.9
A	1091	7447	7413	2507
β	38178	34717	28777	37589

The 4 retained clusters correspond to the only solution clusters that are able to survive in the overall population. Other clusters – identified by frequent reclustering – do not survive because the individuals composing them are considered having too poor objective values. QMOO fixes this removal criterion as follows: an individual is considered being "too poor" if all its objective function values are worse than the corresponding limit value \lim_i defined in Equation 4:

$$lim_i = \max(obj_i) + 0.5 * (\max(obj_i) - \min(obj_i)), i = 1, 2, ..., n$$
 (4)

where obj_i is a vector containing all objective values of the living population for the objective function i and n the total number of objective functions.

Figure 4a suggests that some of the identified locally Pareto-optimal solutions are strictly better than others. It should however be kept in mind that the sub-optimal solution clusters contain nevertheless good solutions and that their sub-optimality for the arbitrarily chosen 5-year calibration period is not necessarily confirmed for another time period. This assumption is sustained by the simulation results for the validation period. Figure 4b shows a plot of the Nash values for all retained sets of decision variables for the calibration and the validation period. None of the solution clusters has strictly better Nash-values for both time periods.

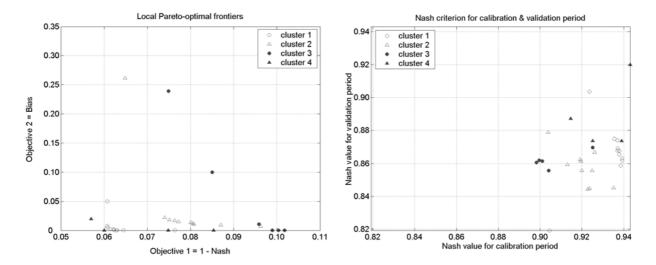


Figure 4:a) Local Pareto-optimal frontiers b) plot of the Nash criterion values for the locally Pareto-optimal sets of decision variables, for calibration and validation period

Figure 4b shows that there is a much wider spread of simulation results for the validation period than for the calibration period. This overall spread is induced by the joint action of all clusters. In a global optimisation approach identifying the global Pareto-optimal frontier, part of the solutions contributing to the spread would not have been retained, as the corresponding individuals would have had to compete with the globally best solutions for the two given objectives.

Model application to future climate scenario

The difference in model performance for distinct time periods is essentially due to the different climatic conditions prevailing during these periods. In the context of the present study, we are particularly interested in the model behaviour under future climate scenarios. We have simulated the future scenario discharge for all retained sets of decision variables and averaged the corresponding simulation results for each cluster. Figure 5 shows the mean monthly results for the discharge, spatially averaged precipitation, liquid precipitation and snowmelt. There is an important difference, not only in the total annual discharge volume but also in the distribution over the year. The differences in the distribution are due to the model structures and the corresponding model parameters, whereas the differences in the discharge volume are due to the altitudinal interpolation of precipitation. For the current situation, this interpolation is balanced by ice melt. For the future scenario, the glacier surface area has drastically reduced. The total runoff volume and the distribution between the different types of runoff contributions are therefore modified. Consequently, the different model structures lead to quite distinct discharge distributions throughout the year.

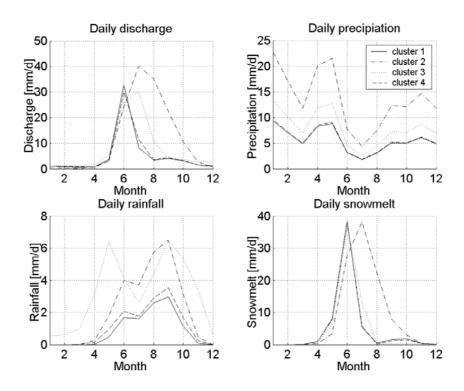


Figure 5: Interannual monthly mean discharge, precipitation, rainfall and snowmelt simulated for the future scenario, average values of the decision variables of each cluster

7. Discussion

The application of QMOO to the presented hydrological model led to the identification of 4 different model structures with equivalent results for the given objective functions and over the given calibration and validation time period. For the future time period however, the retained locally Pareto-optimal solutions sets give considerably different discharge simulations. In a classical hydrological modelling approach, the calibration period should be chosen carefully in order to be representative of the current climate and the robustness of the optimisation results in regard to the time period should be assessed. In the context of climate change impact studies, we are inevitably confronted with the extrapolation of modelling results beyond the domain of validity of the model development and we are thus not able to choose a calibration period representative for the future unknown climate and hydrological conditions. The present study showed that the uncertainty due to the model structure could contribute substantially to the overall modelling uncertainty. Even if its relative importance compared to the parameter estimation uncertainty for a given model set-up cannot be judged here, the uncertainty inherent to the model structure should not be omitted in studies dealing with quantification of modelling uncertainty and climate change impact. Introducing more objective functions could potentially reduce the overall modelling uncertainty. One could especially think of using observed values for some internal model processes to constrain the optimisation solutions. In the context of conceptual modelling, most of the internal variables have however no physical meaning.

We could have chosen to include many other model design options into the optimisation procedure. The presented options correspond to the basic features that could easily be implemented under the given modelling constraints and considering the data availability for future climate scenarios. We therefore do not pretend to cover the whole possible range of model structure uncertainty. The presented case study should rather be considered as an illustration of how to include the model structure efficiently in a model optimisation procedure. For the presented 8 different model set-ups, the joint optimisation of model parameters and structure is around 6 times faster than separate optimisation of each of the model structures (for each model structure, convergence is reached after 6000 to 8000 model evaluations). This

computational gain can become quite important if the number of design decision variables and the corresponding possible values increases. Especially if the total number of possible model structures only includes a few competitive structures, a classic approach optimising each model structure represents an important waste of computational resources. Furthermore the QMOO algorithm yields ready-to-use solutions and there is no need for the user to proceed to additional analyses of the solutions.

8. Conclusions

The present paper illustrates two important aspects for future hydrological research. First, it shows the benefits that hydrological modelling can experience from collaboration with other disciplines dealing with modelling problems such as - for the present study - industrial energy system design. The presented new generation evolutionary algorithm includes some features that are new in the context of hydrological modelling and that are particularly interesting for the presented problem of model design optimisation. Second, the presented application points out that further research into model structure uncertainty estimation is essential for climate change impact studies. Scientists just started addressing the challenge of estimating the overall modelling uncertainty in the modelling chain beginning with global emission scenarios, global and regional climate models and ending in local or regional hydrological models and corresponding impact models. The presented case study in the Swiss Alps shows that for such long-term projections (typically between 50 and 100 years) in non-stationary conditions, the model structure induces uncertainties that are potentially higher than the uncertainty due to the parameter estimation for a given model structure. The combination of our current results with an appropriate methodology for quantitative parameter uncertainty estimation – such as the one applied by (Kuczera and Parent, 1998) - could lead to a good estimate of the overall hydrological modelling uncertainty.

Acknowledgements

We wish to thank Dr. François Maréchal from LENI for having made available the source code of the algorithm QMOO and Dr. Geoff Leyland for its help on the algorithm application and on some theoretical optimisation aspects. The hydrological model has been developed in the context of the European research project SWURVE (Sustainable Water: Uncertainty, Risk and Vulnerability in Europe) that provided the climate change scenario for our case study. The discharge data was provided by the Swiss Federal Office of Hydrology and Geology and the meteorological time series were made available by the national weather service MeteoSwiss. We also wish to thank the anonymous reviewers for their helpful comments.

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