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Hydrological model parameterising using various automatic calibration techniques

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ABSTRACT

Hydrological models are used for various water resources application. To represent hydrological processes, it need parameters that achieve a discharge simulation as close to the observed series as possible. The simulation result depends on how accurately the models parameters are calibrated. The calibration of model parameters depend on various factors, such as calibration methods and selected objective functions. In this study, some of the automatic calibration methods were investigated and a comparison was made to give better prediction. Different optimization algorithms like SCE-UA, SA, and ROPE were used to illustrate and calibrate the conceptual model HBV-IWS. The study was conducted on the Upper Neckar catchment, Germany. The results show that almost all optimization algorithms gave a very similar result, but the ROPE algorithm seems to be more robust. This is due to ROPE giving a space of parameter values after calibration, instead of a single parameter set as in other optimizations.

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1. Introduction

Hydrology is the continuous process of circulation of water, i.e. the water cycle that occurs on Earth. Temperature and precipitation are the two important variables within this process, that mainly contribute to runoff which accumulates as discharge in rivers. Determining the amount of discharge primarily depends on the availability of the observation series. A catchment with a better gauging over a long period of time will give a better estimation of the amount of discharge compared to a catchment that has a lack of data. However, determining the amount of discharge is not a simple process due to many parameters that are involved in the catchment, such as soil properties, infiltration rate, lag time, and others. In order to solve the problems that are related to the rainfall-runoff scheme, hydrological models are used to describe the relationship of these schemes and simplify the complex process in nature into the mathematical forms.

Hydrological models are used for a variety of water resource development activities such as agricultural water consumption (Yu et al., 2015), watershed development (Singh et al., 1999), flow forecasting (Nicolle et al., 2014) and others. In addition, it also can be used for gap-filling streamflow data, particularly when the missing data rate is less than 10%, as studied by Zhang and Post (2018). Generally, there are three types of hydrological models that exist: conceptual model, physically-based model, and empirical model. Each of these kinds of models have advantages and disadvantages that depend on the case that needs to be solved. There are several models that are usually used to describe the behavior of rainfall-runoff process, such as HBV, HYMOD, Tank model, TOPMODEL, VIC, SACRAMENTO, mHM and others. For modeling the rainfall-runoff process, various models have been developed that are based on conceptual representations of the physical processes of the water flow lumped over the entire catchment area (lumped conceptual type of models).

These need some parameters in order to achieve the result that will match the observed series as closely as possible. Besides temperature and precipitation, other variables are also taken into consideration for particular hydrological models (e.g., initial groundwater table, soil moisture).

The great difficulty in modeling is parameterization which is the process to achieve the value that makes the model as close to the observed series as possible. Currently, there are few methods of parameter calibration which are divided into two categories, namely manual and automatic calibration. Generally defined, manual calibration is done manually and needs extremely complete information and the process of the model.

In addition, it is used by those who have geological expertise and have extensive experience in hydrology, and thus, manual calibration is time-consuming (Lee et al., 2006). Meanwhile, automatic calibration depends mainly on an algorithm to find the optimal value of a particular parameter. The main advantage of automatic calibration is that it does not require complete information from nature, and it depends only on certain important parameters.

Most automatic calibrations produce a single value for a particular parameter of hydrological modeling. In other words, chosen a different value without a certain range after calibration will affect the simulation results. This paper is presenting the comparison parameters results in between different automatic calibrations. In this study, different techniques of automatic parameter optimizations were used in order to understand the merit and demerit of each of these methods.

The methods consist of Shuffled Complex Evolution – University of Arizona (Duan et al., 1994), Robust Parameter Estimation (Bárdossy and Singh, 2008), and Simulated Annealing (Kirkpatrick et al., 1983). Each of these automatic calibrations used a different algorithm to get an optimum of a parameter value.

The structure of the paper is the following: the description of the HBV-IWS model and case study are provided in Section 2; Section 3 gives the general description of three different automatic calibrations; the results are discussed in Section 4.

2. Material and Methods

2.1. Hydrological Modeling

There are many types of conceptual hydrological models (e.g. TOPMODEL, HBV) that have been developed in different regions and climatic conditions. However, among these models, HBV gives satisfactory results (Gayathri et al., 2015) in describing the relationship between the rainfall and runoff processes. In this study, the HBV-IWS model has been used to determine the relationship between rainfall-runoff processes through the parameter calibration. The HBV model is a conceptual model that was first introduced by the Swedish Meteorological and Hydrological Institute (SMHI) in the early 1970's. It is predominantly used in Scandinavia and in other parts of Europe (Addor & Melsen, 2019). Furthermore, this model has been modified in some versions. The Institute of Hydraulic Engineering (IWS), University of Stuttgart has modified the HBV, which includes the conceptual routines for calculating snow accumulation and melts, soil moisture and runoff generation, a runoff concentration within the sub-catchment, and flood routing of the discharge in the river network (Bárdossy and Singh, 2008). Figure 1 shows the HBV-IWS model structure.

A general description of the main parts of the modified version is as follows:

Snow accumulation and melt routine

In this process, a certain value of a threshold temperature (TT) was used to determine the type of precipitation. If a temperature value (T) is below TT, then precipitation falls down as snow which leads to snow accumulation. In contrast, if a temperature value is above TT, then precipitation falls down as rain and the accumulated snow is melted which is calculated with a degree-day (DD) approach as set out in Equation 1.

$$MELT = DD.(T - TT) \quad (1)$$

with, DD is a degree-day factor ($mm^0C^{-1}day^{-1}$). Furthermore, these values DD and TT will be determined by the calibration process.

Soil moisture accounting

Soil moisture was calculated by balancing the precipitation and evapotranspiration using the field capacity and permanent wilting point as parameters (Bárdossy & Singh, 2008), as set out in Equation 2 to 5.

$$P_{eff} = \left(\frac{SM}{FC} \right)^{\beta} .(P + MELT) \quad (2)$$

$$PE_A = (1 + C_E \,.\, (T - T_M)).PE_M \quad (3)$$

$$\text{if } SM \geq PWP, \quad E_A = PE_A \quad (4)$$

$$\text{if } SM < PWP, \quad E_A = \left(\frac{SM}{PWP} \right).PE_A \quad (5)$$

with, P_{eff} = effective precipitation (mm);
SM = soil moisture (mm);
FC = field capacity (maximal amount of water the soil can hold) (mm);
β = parameter in soil moisture routine;
P = precipitation depth (mm);
$MELT$ = melting snow depth (mm);
PE_A = potential evapotranspiration (mm);
C_E = parameter in evapotranspiration routine ($^{\circ}C^{-1}$);
T = mean temperature ($^{\circ}C$);
T_M = mean monthly temperature ($^{\circ}C$);
PE_M = monthly averaged potential evapotranspiration (mm);
PWP = permanent wilting point (limit for potential evapotranspiration) (mm);
E_A = actual evapotranspiration (mm).

Runoff response routing

It considers the flow that consists of surface runoff, interflow, percolation, and groundwater flow also known as base flow. This runoff analysis was calculated using the following equations.

$$Q_0 = k_0 .(S_1 - L).A \quad (6)$$

$$Q_1 = k_1 .S_1 .A \quad (7)$$

$$Q_{perc} = k_{perc} .S_1 .A \quad (8)$$

$$Q_2 = k_2 .S_2 .A \quad (9)$$

with, Q_0 = surface runoff (m^3/s);
Q_1 = interflow (m^3/s);
Q_{perc} = percolation (m^3/s);
Q_2 = groundwater flow or base flow (m^3/s);
A = catchment area (km^2);
k_0 = storage constant for upper reservoir, upper outlet;
k_1 = storage constant for upper reservoir, lower outlet;
k_{perc} = storage constant for percolation from upper to lower reservoir;
k_2 = storage constant for lower reservoir;
S_1 =water level in the upper catchment reservoir (mm);
S_2 = water level in the lower catchment reservoir (mm);
L = threshold water depth in the upper reservoir (mm).

2.2. Study Area

The study was conducted on the Upper Neckar catchment, located in southwest Germany (Fig. 2). The study area elevation has a range in between 241 to 1010 metres above mean sea level (Fig. 3). The Neckar catchment has a total area of 4000 km^2 and is divided into 13 sub-catchments (Table 1). Further details about the location, please refer to Bárdossy and Das (2008); Bárdossy and Singh (2008). In this study, daily discharge series from a sub-catchment Rottweil during the period 1961 - 1970 was chosen to illustrate the comparison of three different calibration methods.

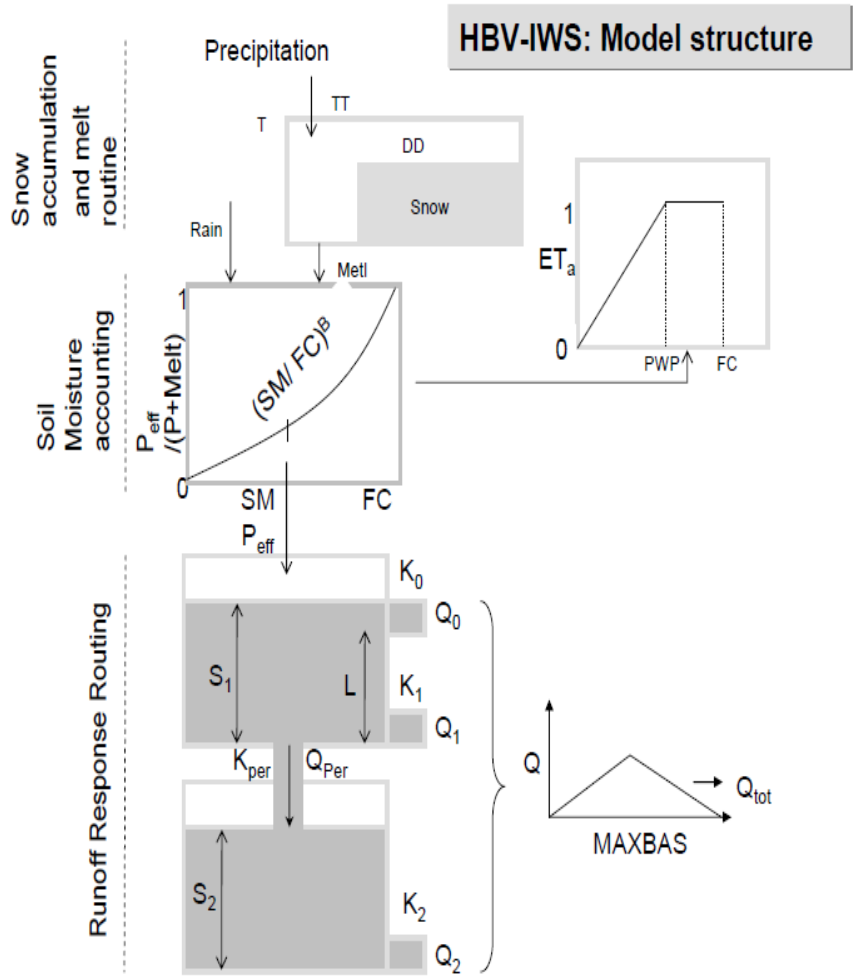

Fig. 1. HBV-IWS model structure

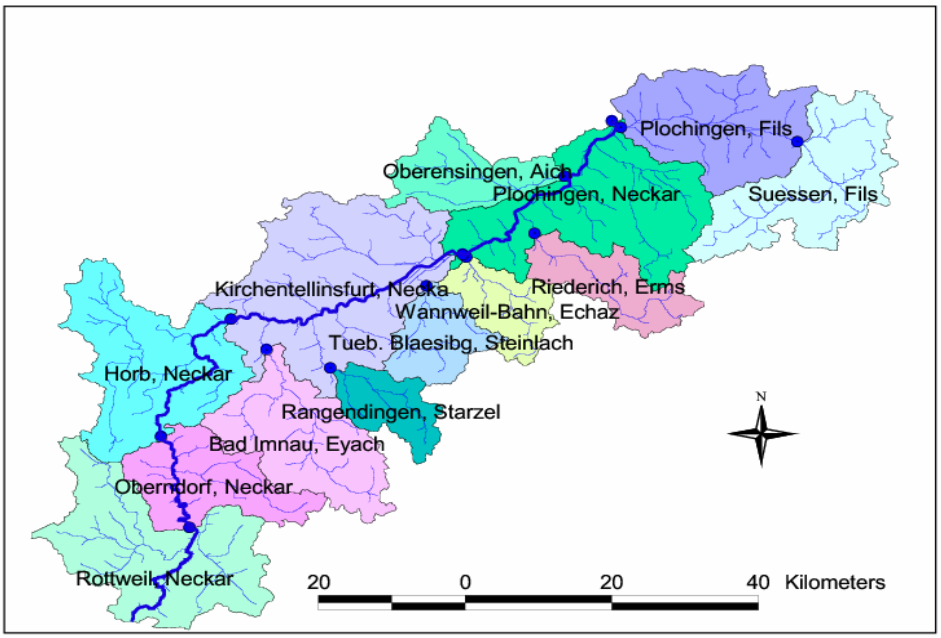

Fig. 2. Neckar catchment area

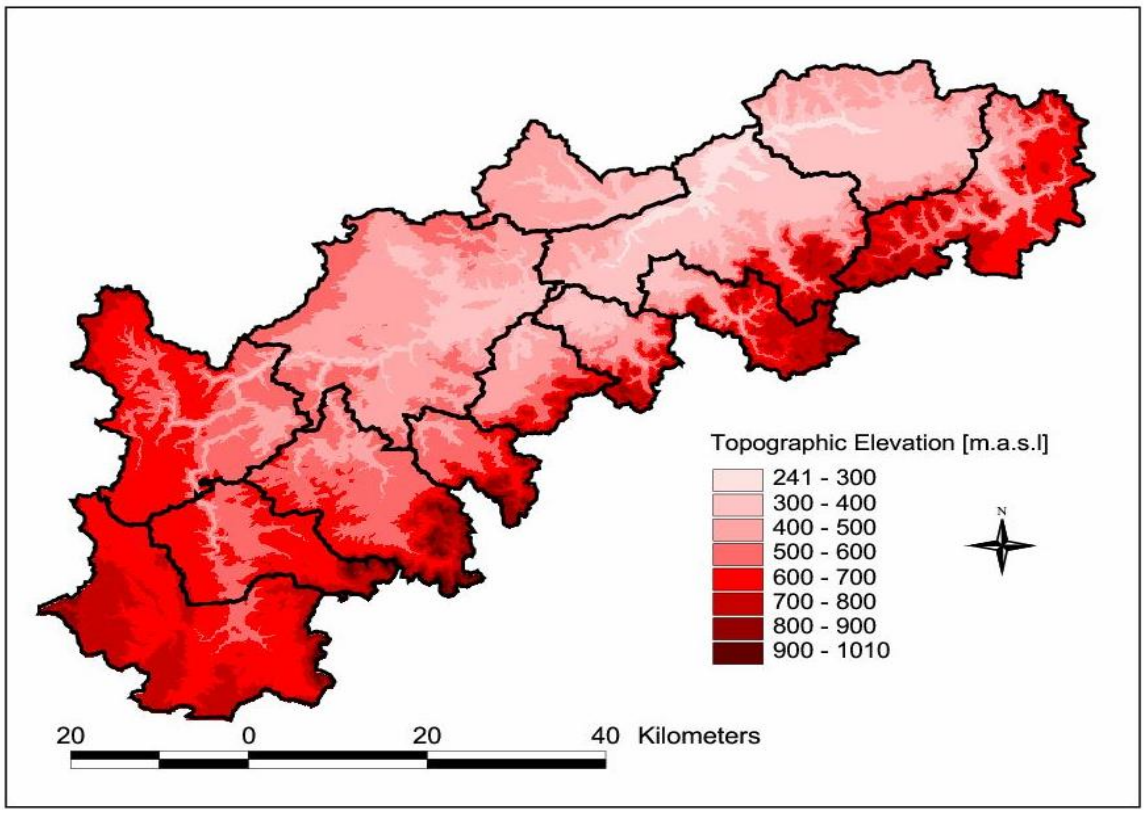

Fig. 3. Elevation of neckar catchment

Table 1. Neckar catchment area

No	Subcatchment	Subcatchment size (km^2)	Elevation (m)	Mean Discharge (m^3/s)
1	Rottweil	456	555-1010	5.1
2	Oberndorf	235	460-1004	7.9
3	Horb	427	383-841	14.8
4	Bad Imnau, Eyach	323	394-988	3.4
5	Rangendingen, Starzel	118	421-954	1.3
6	Tuebingen, Steinlach	140	341-882	1.7
7	Kirchentellinsfurt	618	308-622	46.6
8	Wannweil, Echaz	135	309-862	2.8
9	Riederich, Erms	170	317-865	3.0
10	Oberensingen, Aich	175	278-601	1.3
11	Suessen, Fils	340	359-859	5.9
12	Plochingen, Fils	352	252-785	9.8
13	Plochingen, Neckar	473	241-871	49.9

2.3. Model Calibration

In order to get the simulation result as close to the observation series as possible, the model algorithm should be both logical and physically relevant, and the model should simulate as accurately as possible the streamflow hydrograph (Bergstrom and Forsman, 1973). In other words, hydrological models need parameters to achieve an accurate simulation of discharge that is as close as the observed series as possible. In order to have a close match with the observed series, parameters in hydrological model need to be calibrated. According to Gupta et al. (1999), the usefulness of hydrologic models for the purpose of operational predictions depends on how well the models are calibrated. The conceptual model generally has a large number of parameters which are not directly measurable and therefore must be estimated through model calibration, i.e. by fitting the simulated outputs of the model to the observed outputs of the watershed by adjusting the model parameters (Duan et al., 1994). In addition, to calibrate a hydrologic model, the hydrologist must specify values for its parameters in such a way that the model's behavior closely matches that of the real system it represents (Yapo et al., 1998). A measure of the fit between the simulated and observed outputs is called a calibration criterion or objective function (Duan et al., 1994). In this study, the model performance or objective function will be examined using the Nash-Sutcliffe (NS) coefficient. Related to the calibration, in general it consists of manual and automatic calibrations. According to Lee et al. (2006), manual calibration is mainly needed a comprehensive understanding of the catchment runoff behavior, the model structure and can be extremely time-consuming. Meanwhile, automatic calibration involves the use of a search algorithm to determine the best-fit parameters, and it offers a number of advantages over the manual approach with respect to calibration running time and extensive search of the existing parameter possibilities (Lee et al., 2006). Furthermore, the goal of calibration is to find those values for the model parameters that minimize or maximize the specified calibration criterion (Duan et al., 1994). Different techniques of calibration will give different parameter values. There are many types of automatic calibration in hydrological modeling, and in this study, three different selected automatic calibrations were used. It consists of SCE-UA, SA, and ROPE. The general description of each algorithm is as follows:

Shuffled complex evolution – University of Arizona (SCE-UA)

The SCE-UA method (Duan et al., 1993) was used in this study to obtain the parameter values for the simulated discharge of the HBV-IWS model. According to Yapo et al. (1996), SCE-UA is a general purpose of a global optimization strategy designed to handle the various response surface problems encountered in the calibration of non-linear simulation models. In addition, this method is a probabilistic global search method which is intended to combine the strength of the simplex search with the concepts of controlled random search, competitive evolution, and shuffling of complexes or communities (Goswami & O'Connor, 2007).

The SCE algorithm involves the following steps (Duan et al., 1993; Madsen et al., 2002):

An initial sample of parameter sets is randomly generated from the feasible parameter space. Furthermore, the sample is partitioned into several complexes based on the objective function values of the evaluated parameter sets. Each complex is then evolved independently according to the simplex method. This is a method used to describe for the minimization of a function of n variables, which depends on the comparison of function values at the $(n + 1)$ vertices of a general simplex, followed by the replacement of the vertex with the highest value by another point. Furthermore, the next step, the evolved complexes are shuffled to enable the sharing of information and new complexes are formed.

For more details about the SCE-UA method, please refer to Duan et al., 1993; Lee et al., 2006; Duan et al., 1994. Figure 4 shows the flow chart of the SCE-UA algorithm. In addition, implementation of the SCE-UA method requires the selection of an objective function to be optimized with respect to the model parameters (Gupta et al., 1999).

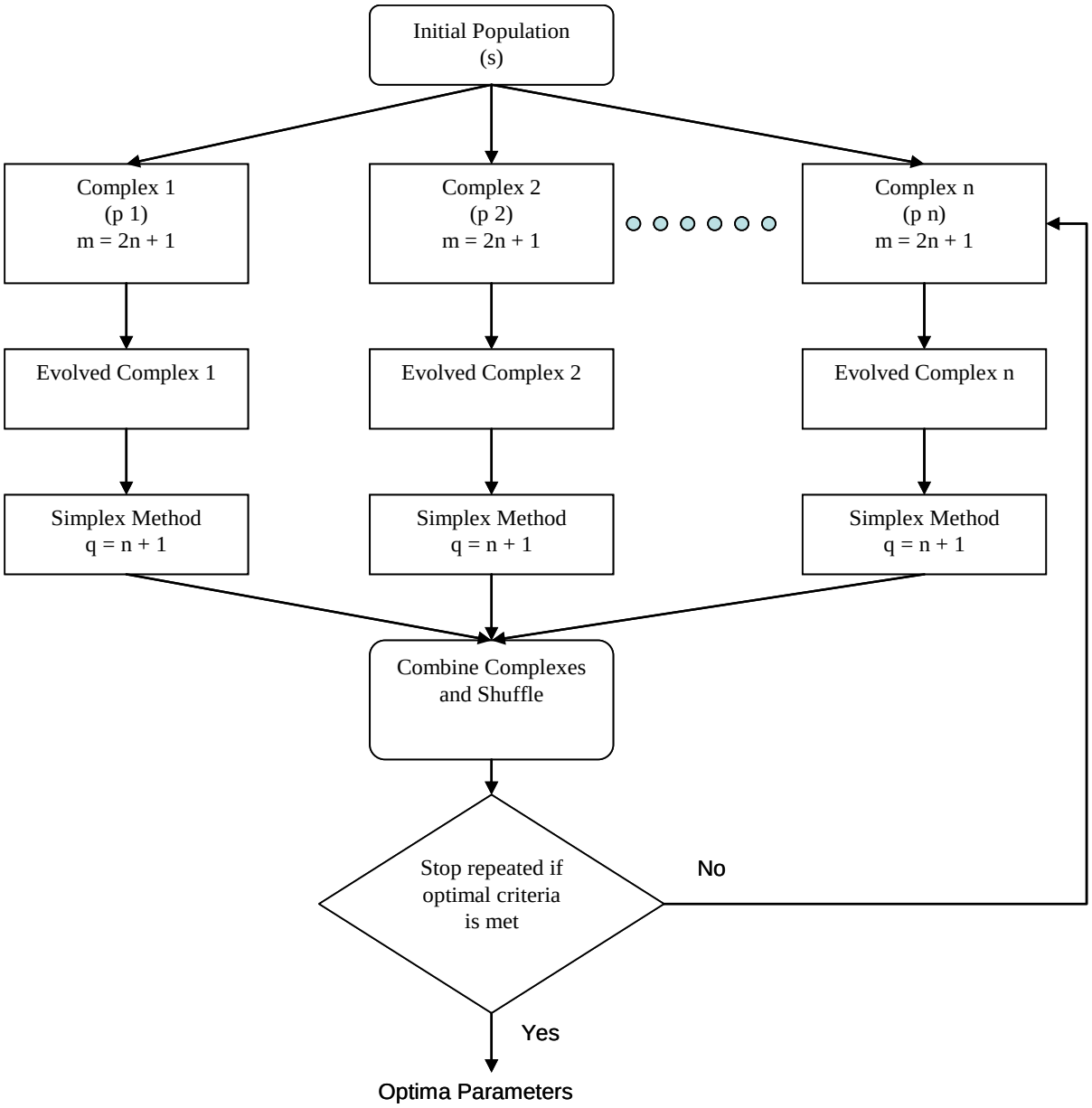

Fig. 4. The algorithm of shuffled complex evolution – university of arizona (SCE- UA)

Simulated Annealing (SA)

Simulated annealing (Kirkpatrick et al., 1983) is a global optimization method that mimics the behavior of a slow cooling solid in a heated bath (Rucker and Ferré, 2005). In addition, it is analogous to the physical annealing process whereby a material is heated to a temperature below its melting point and then cooled slowly to allow the molecules to align themselves, crystallize and attain a minimum energy state (Sumner et al., 1997). The algorithm of SA is depicted in Figure 5.

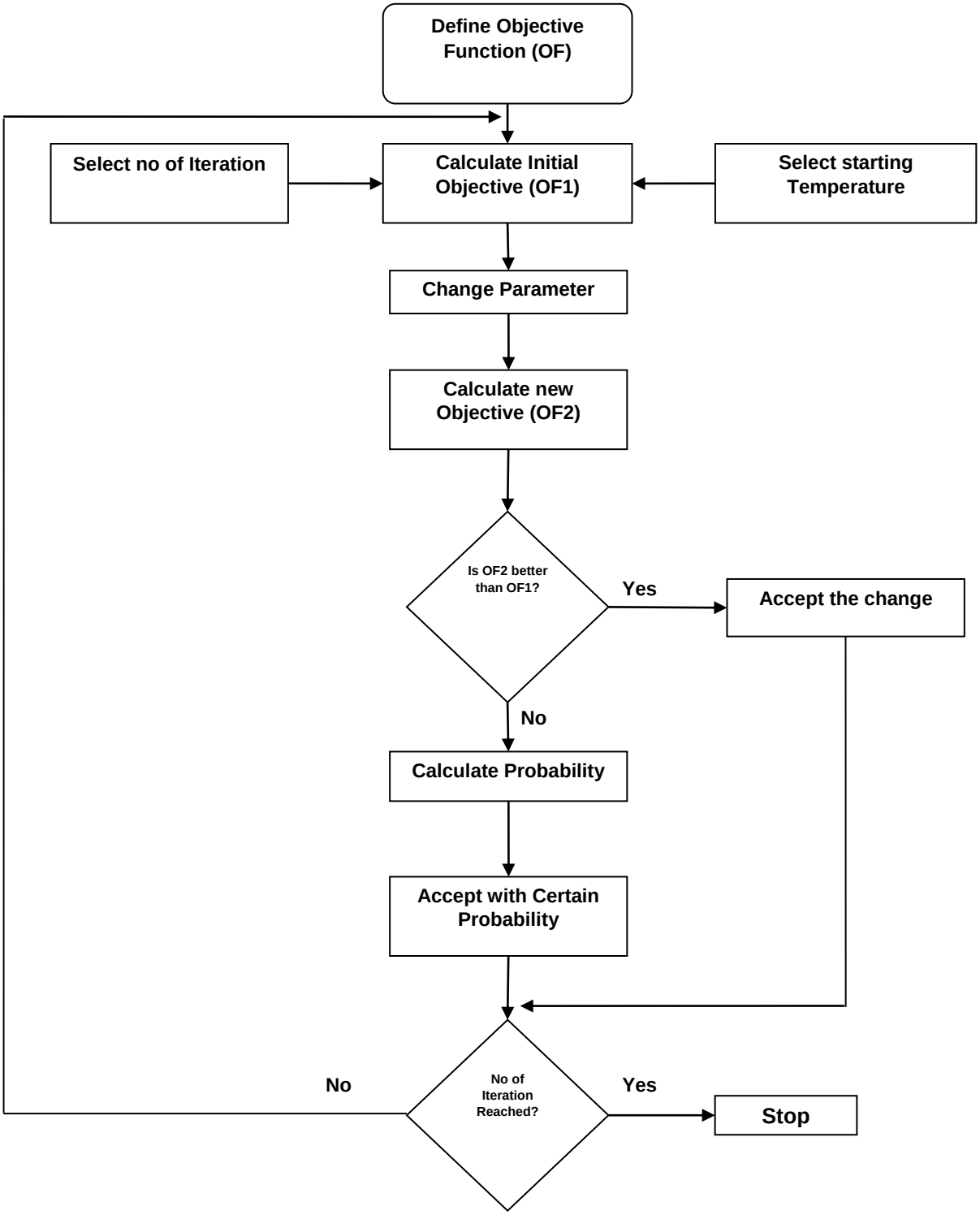

Fig. 5. The algorithm of simulated annealing

In general, this automatic optimization is a random-search technique that is based on the choosing of the objective function. The simulated annealing algorithm starts with a random parameter. Each iteration forms a random nearby solution. If this solution is a better solution (has a new objective function), then it will replace the existing solution. If it is a worse solution, it may be chosen to replace the existing solution with a certain probability that depends on the difference between the initial objective functions. The process will be continued until it reaches the sufficient of iterations.

Robust parameter estimation (ROPE)

Robust parameter estimation (Bárdossy and Singh, 2008) used the concept of data depth function in the parameters optimization. A depth function is a quantitative measurement of how central a point is with respect to a data set (Tukey, 1975). In a general illustration, the highest depth value is located at the center of the data set and low depth values are located at the boundary of the data set. Choosing a depth value is a critical point here, where low depth values correspond to a weak parameter value which affects the calibration results. Figure 6 illustrates the algorithm of ROPE.

The idea of the ROPE algorithm (Bárdossy and Singh, 2008) can be described as follows:

A large set of parameters (maximum and minimum range of parameters) is generated as shown in Figure 6 (a). The model runs for all the parameters and the best 10% parameters are selected (Fig. 6 (b)). After removing the parameter outside the boundary as shown in Figure 6 (c), another set of the same number of parameters is generated in such a way that has higher depth value and located within the boundary space as shown in Figure 6 (d). Thus, as the model is running, the performance of parameter criteria is calculated, and the best 10% parameters are selected. This iteration is continued (Fig. 6(e)) until the predetermined number of iterations is over or the variation in performance is within a selected range (Fig. 6(f)).

There are different types of depth function and in this study, the half-space depth function (Tukey, 1975) was used. This is because it satisfies all four properties of the data depth function as mentioned in Liu (1990).

Objective Function

A hydrological model is calibrated by comparing the observed data series and the model (Diskin and Simon, 1977). There are many different objective functions that can be used to determine the performance of the models compared to observed data (e.g. root mean squared error, correlation coefficient, sum of squared deviation, peak error), and the typical objective function that is used in hydrological model is the Nash-Sutcliffe coefficient (Nash & Sutcliffe, 1970).

$$R_m^2 = 1 - \frac{\sum_{i=i}^{N} \left(Q_o(t_i) - Q_s(t_i)\right)^2}{\sum_{i=1}^{N} \left(Q_o(t_i) - \bar{Q}_o\right)^2} \quad (10)$$

with, R_m^2 = Nash-Sutcliffe coefficient (-);

$Q_o(t_i)$ = observed discharge (m^3/s);

$Q_s(t_i)$ = simulated discharge (m^3/s);

$\bar{Q}_o$ = mean observed discharge (m^3/s);

N = number of time steps.

R_m^2 can range from $-\infty$ to 1 (a perfect match between observation and simulation). An efficiency of lower than zero indicates that the mean value of the observed time series would have been a better predictor than the model (Krause et al., 2005). Furthermore, the Nash-Sutcliffe coefficient leads to a good estimation of model performance during the peak flow and the Nash-Sutcliffe with a logarithmic function gives a good estimation during the low flow.

3. Results and discussion

Three different selected automatic calibrations were investigated in this study in order to compare and determine which one shows the most reliable result based on the objective function value. Table 2 shows eight parameters that were used for the calibration. These parameters were chosen due to the sensitivity and dominant process in hydrological modeling HBV-IWS. Furthermore, all three automatic calibrations used the same initial parameter value for lower and upper boundaries.

Table 2. Parameters selected for calibration using HBV-IWS

No		Parameter	Unit
1	L	Depth of upper reservoir	mm
2	K0	Surface flow storage constant	1/d
3	K1	Interflow storage constant	1/d
4	K2	Baseflow storage constant	1/d
5	KPER	Percolation storage constant	1/d
6	TT	Threshold temperature	^{0}C
7	DD	Degree day factor	mm/^{0}C d
8	β	Model parameter	-

SCE-UA

This method uses two numbers of the complexes and the optimization of parameters is completed when the criterion value has not been changed. All the parameter values after the calibration fall as a single value in between the initial values, as shown in Table 3. Furthermore, Table 4 shows the statistical descriptive result of the observed and model discharge series for the Rottweil sub-catchment. One can clearly observe that a model performance in a mean value is higher by 0.34 m^3/s than in the observation. Meanwhile, for standard deviation, it shows 0.90 m^3/s lower in the model than in the observation, as shown in Table 4.

Table 3. Optimal parameter values with SCE-UA

Parameter	Initial Parameter Value		Value
	Lower Boundary	Upper Boundary	
L	1	40	14.90
K0	0.5	20	0.92
K1	5	50	5.69
K2	10	1000	999.46
Kper	20	100	20.01
TT	-1	1	-0.72
DD	1	3	1.58
β	1	6	1.09

Table 4. Statistical descriptive result using SCE-UA

Sub. Catchment	Obsv. Mean (m^3/s)	Obsv. Std (m^3/s)	Mod. Mean (m^3/s)	Mod. Std (m^3/s)	**NS**
Rottweil	5.42	6.93	5.76	6.03	**0.70**

SA

In order to get a reasonable parameter value, this calibration method uses an objective function of random parameters that will be replaced with the new objective function. The same numbers of parameters with other optimization approaches were used in this method. The optimal value as the result of a model performance gives a single value based on the criterion of the lower and upper boundaries. Table 5 shows the optimal parameter values which fall in between the lower and upper values. Furthermore, Table 6 shows the statistical results from this calibration method. It shows that in the mean value, the model has 0.09 m^3/s higher than the observed discharge. However, in the standard deviation, the observed discharge was higher than the model discharge.

Table 5. Optimal parameter values with SA

Parameter	Initial Parameter Value		Value
	Lower Boundary	Upper Boundary	
L	1	40	11.20
K0	0.5	20	1.59
K1	5	50	6.50
K2	10	1000	169.30
Kper	20	100	20.43
TT	-1	1	0.40
DD	1	3	2.48
β	1	6	1.01

Table 6. Statistical descriptive result using SA

Sub. Catchment	Obsv. Mean (m^3/s)	Obsv. Std (m^3/s)	Mod. Mean (m^3/s)	Mod. Std (m^3/s)	**NS**
Rottweil	5.42	6.93	5.51	6.23	**0.72**

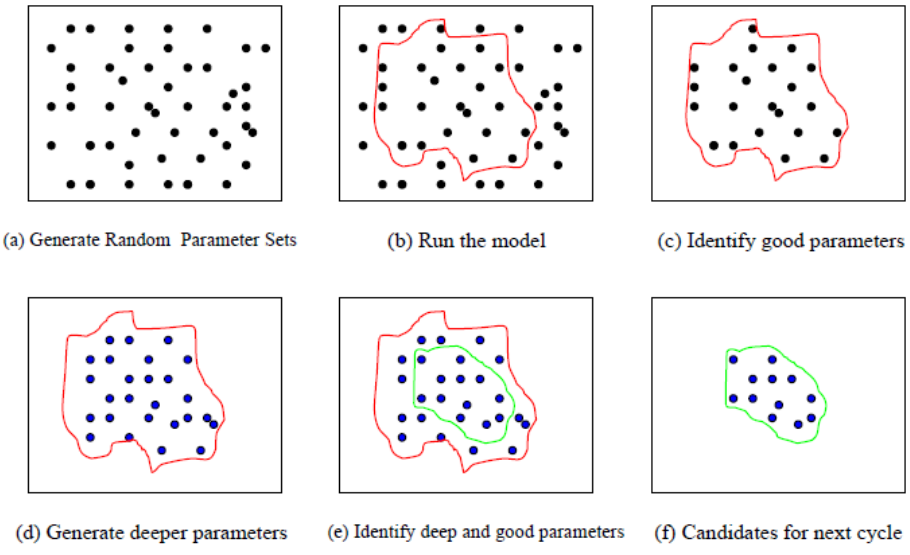

Fig. 6. The algorithm of robust parameter estimation (Bárdossy and Singh, 2008)

ROPE

This method is based on choosing the best parameter sets in each time step within the boundary space. It starts with generating the random parameter and is used for a further iteration until a model produced is close to the observation. In this analysis, the ROPE method starts with generating 10000 random parameters and continues by identifying a good parameter using the concept of the depth function. This method is continued with a four-time step iteration in order to find a good set of parameters. As described before in Section 3 about the algorithm for choosing the best parameter sets, the results are given within the range of maximum and minimum values, instead of a single value. These results are based on the monotonic function having by the depth function in classifying the depth values. It shows the high depth values are located close to the center of the datasets and low depths are located at the boundary of the datasets. Thus, the ROPE gives a space of parameters after calibration based on the ranges of the 'deepest' depth values. The result of ROPE method is shown in Table 7. It is clearly shown that each parameter has their own ranges between maximum and minimum values and they are fall in between the lower and upper boundaries. In addition, it is interesting to note that some parameter values from SCE-UA and SA are located in between maxima and minima values of ROPE after calibrations. This can be seen, for instance, at parameter K1, as depicted in Figure 7.

Table 7. Optimal parameter values with ROPE

Parameter	Initial Parameter Value		Value		
	Lower Boundary	Upper Boundary	max	min	std
L	1	40	18.72	5.56	2.40
K0	0.5	20	6.84	2.02	0.67
K1	5	50	44.57	5.15	7.75
K2	10	1000	838.99	199.61	118.25
Kper	20	100	89.09	34.32	9.79
TT	-1	1	0.49	-0.55	0.15
DD	1	3	2.72	1.42	0.23
β	1	6	1.41	1.02	0.07

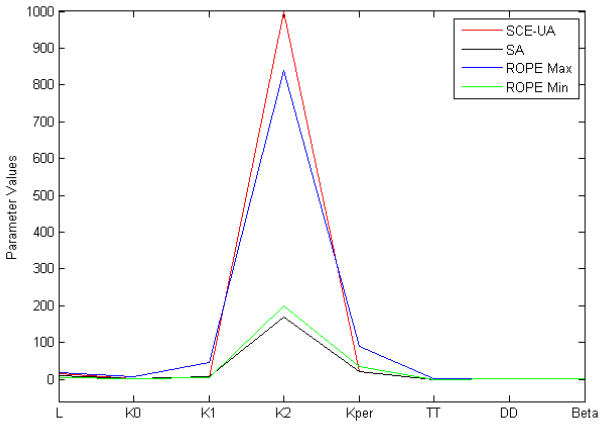

Fig. 7. Model parameter values from different automatic calibrations

Related to the statistical descriptive of this method, Table 8 shows the observed discharge with 5.42 m^3/s is located in between the maxima and minima model values, 6.48 m^3/s and 3.42 m^3/s, respectively. The same thing is applied to the standard deviation value. In the context of the objective function R_m^2 (see Table 8), SA shows closer to the observed series with a coefficient of 0.72, followed by SCE-UA (0.70) and ROPE (0.69). However, for the first two optimizations, the model parameters have no option to choose any other value, instead of a single value obtained from the calibration. Meanwhile, ROPE gives the flexibility of choosing any parameter values that range in between maxima and minima values. In other words, choosing any value within these ranges or space of parameter values, will not influence a significant change in the objective function. Thus, the model discharge will have confidence in interval values. Table 9 shows the highest and lowest discharge series in Rottweil with 114.64 m^3/s and 0.45 m^3/s, respectively. For the first discharge, it shows that all optimization techniques have the highest model discharges which are smaller than in the observed series for the period 1961 – 1970. Meanwhile, for the lowest discharge, it shows that ROPE has the smallest value of 0.22 m^3/s compared to the other two techniques and observation. The hydrograph between the observed discharge series and discharge simulation from three different automatic calibrations are depicted in Figure 8. One can clearly observe that there are some parts where model perform well with the observed series and others perform less, particularly for the peak flow. The possible reasons of this situation might be caused by the numbers of sensitivity parameters, the input values, and the model structure itself. In addition, Figure 8 shows of how closely the observation series and model. The calibration of model parameters through SCE-UA and SA give over and under estimate of the model with respect to the observation series. Meanwhile, ROPE gives a good model performance due to maximum and minimum value of a model compared with the observed discharge series. In other words, in general, it shows that the observed series are located in between the maximum and minimum of the discharge simulation (model). This calibration analysis is indicating a promising result of analysis and shows a good estimation and performance of the model parameter values.

Table 8. Statistical descriptive result using ROPE

Sub. Catchment	Obsv. Mean (m^3/s)	Obsv. Std (m^3/s)	Mod. Max (m^3/s)	Mod. Std Max (m^3/s)	Mod. Min (m^3/s)	Mod. Std Min (m^3/s)	NS		
							Max	Min	Mean
Rottweil	5.42	6.93	6.48	7.25	3.42	4.53	0.70	0.67	0.69

Table 9. Highest and lowest discharge in sub-catchment Rottweil period 1961-1970

	Simulation Discharge (m^3/s)		Observation Discharge (m^3/s)
Highest (m^3/s)	SCE-UA	83.27	114.64
	SA	107.7	
	ROPE Max	106.93	
Lowest (m^3/s)	SCE-UA	0.46	0.45
	SA	0.52	
	ROPE Min	0.22	

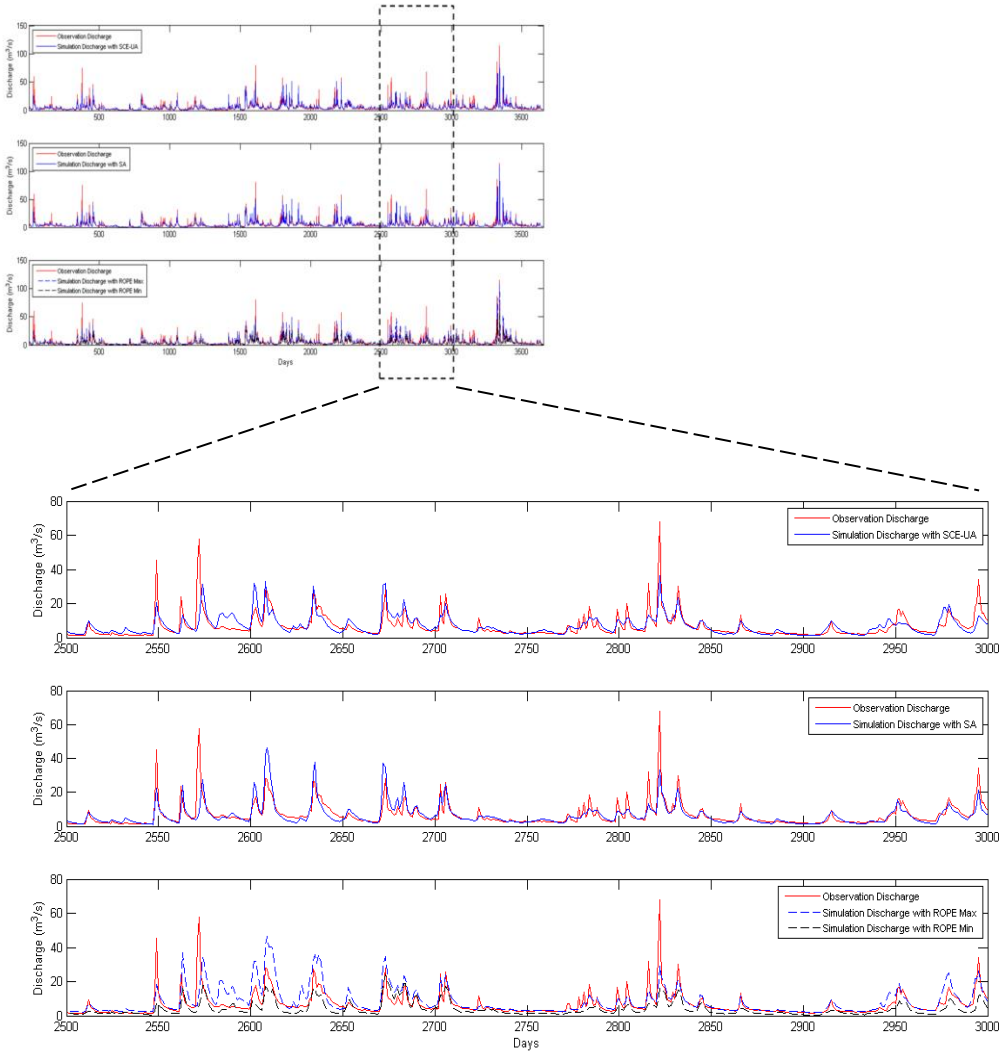

Fig. 8. The hydrographs between the observation and model discharge with different automatic optimization techniques

4. Conclusion

The great difficulty in modeling is parameterization of any model. In this study, different techniques of automatic calibration were used in order to understand the merit and demerit of each of the parameter optimization methods. The study was conducted in the sub-catchment Rottweil that is located in the Upper Neckar catchment, Germany. The result was analyzed to make a strategy for selecting the most accurate optimization of the conceptual model. It has been found that the parameters obtained by different optimization algorithms can result in different parameter sets. The SA method seems to be more effective than the other automatic calibration, due to the Nash-Sutcliffe coefficient indicating a good performance when compared to the observed data. However, the ROPE method seems to be more robust, because this method gives a range of parameters after calibration of the hydrological model, instead of single parameter sets in the others optimization. Furthermore, ROPE can be used to improve the confidence in forecasting because it gives a better approach to the hydrological model.

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