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SWAT model parameter calibration and uncertainty analysis using the HydroPSO R package in Nzoia Basin, Kenya

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Abstract The parameter uncertainty in hydrological modelling has been accorded much attention in the recent past. Parameter uncertainty is a major source of overall model unreliability. In this study, the HydroPSO R package was used to assess parameter identification and uncertainty for the Soil and Water Assessment Tool (SWAT) model applied in the upper reaches of Nzoia River Basin. Fourteen parameters were selected based on previous studies and parameter sensitivity analysis using the Latin Hypercube Sampling method. Based on the optimum parameter set, the simulated flow corresponded well with the observed flow with daily Percent Bias (PBIAS), coefficient of determination (R²) and Nash–Sutcliffe efficiency (NSE) of -1.4, 0.73 and 0.72, respectively. For monthly calibration, these values were -1.4, 0.78 and 0.77, respectively. The results of this study show uncertainty in parameter identification. The posterior distributions of the parameter values were not normally distributed and the uncertainty ranges of the parameters varied widely. The low flows (Q5) were overestimated with a 13.8% bias while the Q50 and Q95 flows were underestimated with -4.2% and -13.1% biases respectively. Further analysis indicated that the contribution of parameter uncertainty to stream flow simulation was substantial with 35% of the observed flow data falling within the 95% simulation confidence interval for the calibration period. Different parameter sets gave the same correlation between the simulated and observed flows. A multiobjective analysis of the hydrological modeling uncertainties emanating from model selection, calibration procedure and calibration data errors in the basin is therefore recommended.

Keywords hydroPSO, parameter identification, uncertainty analysis, Nzoia Basin, hydrological models

1. Introduction

The development of hydrological models of varying nature, complexity and purpose is perhaps an exceptional achievement in the recent past [1]. The simulation of hydrological processes at local, regional and global scales has played a key role in addressing a wide range of environmental, social and water resources management challenges. Despite the growing interest in watershed modeling, uncertainty in model output is still a limitation in the simulation of hydrological processes. The model

selection, calibration procedure, and calibration data errors are major sources of uncertainty [2]–[5].

The improvements data resolution and computational power have contributed development of semi-distributed, physically-based hydrological model, such as the Soil and Water Assessment Tool (SWAT). The models are particularly important tools commonly used in modeling the land phase of the hydrological cycle based on hydrological response units. However, these models consist of a large number of parameters which are generally determined by



calibration due to high cost of field measurements [6]. The spatial-temporal variations in the optimum values of these parameters disclose a substantial amount of uncertainty with dire implications on water resource and watershed management [7], [8]. Thus effective utilization of these models requires robust calibration and uncertainty analysis techniques.

Parameter identification and estimation are two significant steps in model calibration. The former entails identification of sensitive parameters, mainly through a sensitivity analysis, while the latter involves manual or automatic estimation of the optimal or near-optimal values of the sensitive parameters [9]–[12]. These processes are characterized by varying uncertainties leading to overall model parameter uncertainty. For instance, different parameter sets can be used to obtain similarly good fits between observed and simulated stream flow ("equifinality") [13]. In addition, best parameters during the calibration period may not be reliable during other periods. Thus, parameter calibration should not only focus on the optimum parameter value but also its uncertainty.

A wide range of studies have focused on the analysis of parameter uncertainty [3], [8], [14]–[19]. Consequently, a plethora of methods with varied philosophy, sampling strategies and underlying assumptions have been devised to address parameter uncertainty in hydrological modeling. These include Generalized Likelihood Uncertainty Estimation (GLUE) [13], Particle Swarm Optimization (PSO) algorithm [20], Differential Evolution Adaptive Metropolis (DREAM) algorithm [21], Shuffled complex evolution Metropolis algorithm [22], Sequential Uncertainty Fitting (SUFI) [23], Bayesian Total Error Analysis (BATEA) [24] and Parameter solutions (ParaSol) [25]. The population-based global optimization techniques have particularly been used to overcome the fore-mentioned model calibration challenges.

In this paper, the focus was on the application of the HydroPSO R algorithm for SWAT model calibration and parameter uncertainty analysis in Nzoia Basin. PSO is an adaptive population-based stochastic optimization technique which closely resembles evolution-based optimization techniques such as genetic algorithms, and is capable of efficiently estimating best parameter values in highly non-linear and complex applications [20]. The algorithm globally searches the parameter space on the basis of individual and neighborhood-based best-known "particle positions" (coordinates of particles in the parameter space) without evolutionary operators such as mutation or crossover. Thus, each particle in the population adjusts its 'flying' direction and speed

(velocities) in the multidimensional search-space based on its own flying experience (personal best) and that of its companions (global best). In addition, the new position of each particle is determined by adding the new velocity from the achieved best solution to the current position [26]. The algorithm has been used widely in model parameter calibration and uncertainty analysis [27], [28]. It has also been modified into numerous variants ranging from the original PSO procedure to more adaptive versions for improved global optimization and model calibration [29],[30].

The multi-OS and model-independent *hydroPSO* R package developed by Zambrano-Bigiarini and Rojas, [31] was used in this study for SWAT model sensitivity analysis, calibration, and analysis of the results. As one of the most optimized versions of the PSO algorithm, the *hydroPSO* calibration engine combines the benefits of multiple PSO variants and fine-tuning options to enhance flexibility and efficiency in the calibration of different models. This package has shown improved performance in complex response surfaces such as in hydrological modeling applications [31]. A detailed description of the package can be obtained from [31].

2. Study area

The upper reaches of the Nzoia Basin, a catchment in Western Kenya with a drainage area of 10,156 km² was selected for this study (Fig. 1). The area has tropical-humid climate with annual mean rainfall reaching 1400 to 1800 mm and mean temperature ranging from 14 to 24°C. The annual rainfall pattern is bimodal with minimal intra-annual variability. The long and short rains occur between March and June and from September to November respectively. The elevation in the area ranges from 878 m above sea level (m.a.s.l) at the lower point to 4304 m.a.s.l at the peak of Mt. Elgon. The main land use types are forests, bushland, large-scale and small-holder farmland. The weather stations used in this study are shown in Fig. 1.

3. Materials and methods

3.1 SWAT model

SWAT is a physically based, semi-distributed hydrological model developed by the United States Department of Agriculture–Agricultural Research Service (USDA–ARS). It simulates surface runoff (using the SCS curve number or Green and Ampt infiltration equation), percolation, lateral flow, groundwater flow from shallow aquifers to streams, evapotranspiration (using the Hargreaves, Priestley-Taylor or Penman-



Monteith method), transmission losses from streams and water storage, losses from ponds, and snowmelt in watersheds [32],[33]. The watershed hydrology in the SWAT model consists of the land and water or routing phases and is simulated based on the water balance equation (equation 1).

$$SW_t = SW_0 + \sum_{i=1}^t (R_{day} - Q_{surf} - E_a - w_{seep} - Q_{gw})_t$$
(1)

where SW_t (in mm) is the final soil water content; SW_0 (in mm) is the initial soil water content on day i, t (day) is the time; R_{day} (in mm) is the amount of precipitation on day i, Q_{surf} (in mm) is the amount of surface runoff on day i, , E_a (in mm) is the amount of evapotranspiration on day i, w_{seep} (in mm) is the amount of water entering the vadose zone from the soil profile on day i, and Q_{gw} (in mm) is the amount of return flow on day i.

on topography, vegetation, soil properties and weather. A Digital Elevation Model (DEM) with a 90 m resolution was obtained from the NASA Shuttle Radar Topography Mission (SRTM) [34] while a Land cover map of the area was acquired from the Joint Research Centre (JRC) of the European Commission Global Land Cover 2000 dataset [35] and reclassified according to SWAT model input requirements. The Kenya Soil and Terrain database (KENSOTER) [36] was used to derive soil characteristics in the area. Precipitation and temperature data covering the 1970-1998 period were obtained from the Kenya Meteorological Department. The missing values were estimated using the SWAT model weather generator. Daily wind speed and relative humidity data was unavailable for the area hence were simulated using the weather generator. In order to compare simulated data, the daily discharge data for the 1DD01A River gauging station (Latitude 0.37 °N, Longitude 34.49 °E) were obtained from the Water Resource Management Authority (WRMA).

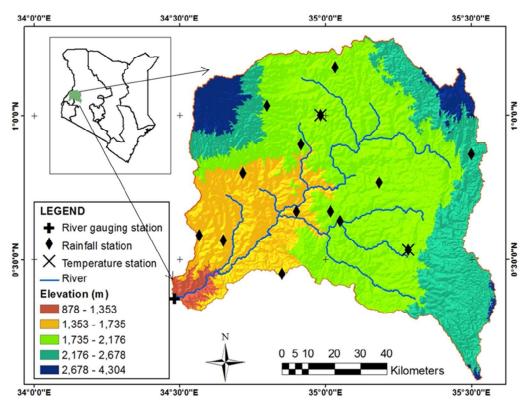


Fig. 1: Location of the study region and hydro-meteorological stations

3.2 Data

3.3 SWAT model set up and parameterization

In order to obtain model parameters in SWAT, a wide range of input datasets is required including, information Using the river gauging station as the main outlet, 17 subbasins were delineated for the Nzoia Basin. Potential



evapo-transpiration was estimated using the Hargreaves method while surface runoff was simulated using the modified Soil Conservation Service (SCS) curve number method. Routing of the surface runoff to river channels was simulated using the variable storage method [32]. Streamflow was simulated using 1984-1985 as model warm-up period and 1986-1990 as calibration period.

Watershed properties in the SWAT model are defined based on a large number of parameters. 14 parameters were selected for calibration in this study based on a literature survey, and results from Latin Hypercube-one factor at a Time (LH-OAT) parameter sensitivity analysis.

Table 1 gives a summary of the selected parameters, calibration value ranges and processes they influence in the water cycle. These parameters correspond to baseflow and surface runoff generation, evaporation, soil types and channel routing. The lower and upper boundaries of the parameter ranges were modified prior to calibration in relation to the default values to ensure sufficient parameter space while at the same time ensuring a fast convergence.

Table 1: Parameters selected for SWAT model calibration

| Name | Definition | Cal. Range | Process |
|----------|--|------------|-------------|
| CN2 | SCS moisture condition II curve number for pervious areas | 40-60 | Runoff |
| ESCO | Soil evaporation compensation coefficient | 0.4-0.8 | Evaporation |
| SURLAG | Surface runoff lag coefficient | 0.05-5 | Runoff |
| RCHRG_DP | Deep aquifer percolation fraction. | 0-1 | Groundwater |
| GWQMN | Threshold water level in shallow aquifer for base flow (mm H ₂ O) | 1200-1900 | Groundwater |
| GW_REVAP | Groundwater "revap" coefficient. | 0.02-0.1 | Groundwater |
| GW_DELAY | Groundwater delay (days) | 45-65 | Groundwater |
| ALPHA_BF | Baseflow recession constant (days) | 0.25-0.65 | Groundwater |
| SOL_K | Saturated hydraulic conductivity (mm/hr) | 10-200 | Runoff |
| EPCO | Plant uptake compensation factor | 0.2-0.6 | ET |
| SOL AWC | Soil available water storage capacity (mm H2O/mm soil) | 0.03-0.30 | Runoff |
| CH N2 | Manning's n value for main channel | 0.016-0.1 | Routing |
| CH_K2 | Effective hydraulic conductivity in main channel alluvium (mm/hr). | 40-80 | Routing |
| OV_N | Manning's "n" value for overland flow | 0.4-0.6 | Runoff |

3.4 HydroPSO setup

The 1986-1990 period was used for model calibration and calculating the goodness of fit between the simulated and observed flow based on the Nash-Sutcliff Efficiency (NSE) objective function. The algorithm was run for 1000 maximum iterations, and 40 swarms of parameter particles. As recommended by Clerc [37], when the search space is not a hypercube parameter values were normalized to the [0,1] range during the optimization. The sampling of the initial particle position and velocity was improved by using Latin hypercube sampling over the full multi-dimensional search-space. The PSO2011 algorithm was used to initialize particle direction and speed as well as maximizing the NSE value.

In order to ensure proper convergence of the algorithm, three parameters were defined namely (i) the constriction factor, (ii) the cognitive acceleration coefficient, and (iii) the social coefficient. The constriction factor is used to prevent an unrestrained increase in the magnitude of velocities which may lead to particle displacement [38]. The cognitive acceleration and social coefficients affect

the balance between the local exploitation and the global exploration search capabilities of the algorithm thus regulate the influence of the personal and the local best [39]. A constant value of 2.05 was used for the cognitive (c1) and social (c2) coefficients. In addition, definition of the factor clamping the velocities (lambda) was improved by using a linear variation between [1.0, 0.5]. The random topology was used to control particle interaction using five informants [37]. In order to confine particles to physically meaningful parameter ranges, a multi-dimensional vector defining the range of the search-space is used in HydroPSO. In this study, the absorbing boundary condition was used, whereby the particle's position is set to the boundary value while the velocity is set to zero [37].

3.5 Model performance evaluation

The HydroPSO package provides a wide range of statistical and graphical techniques to robustly assess the different aspects of the hydrograph for model performance evaluation. Three statistical criteria were selected in this study: the Nash–Sutcliffe efficiency



(NSE), the coefficient of determination (R^2) and Percent Bias (PBias). The NSE measures the model efficiency as a fraction of the measured stream flow variance reproduced by the model in replicating individual values [40]. It is therefore a normalized statistic, ranging between - ∞ and 1, which determines the relative magnitude of the residual variance compared to the measured data variance. NSE values between 0.75 and 0.36 are considered satisfactory while values \ge 0.75 are considered excellent [40].

The R^2 measures the degree of co-linearity between simulated and measured values and ranges from 0 to 1, whereby values greater than 0.5 are generally considered acceptable [41]. PBias measures the percentage difference between the simulated and measured values. A positive (negative) PBias value indicates model underestimation (overestimation) bias while the optimal value is zero. PBIAS values $<\pm25$ % are considered satisfactory [41].

4. Results and Discussion

4.1 Model calibration

The global best parameter set was used to run the SWAT model for calibration performance evaluation.

The Kling-Gupta efficiency (KGE) metric introduced by Gupta et al. [42] was also used to circumvent the limitation of squared differences in NSE. The KGE values also indicated good performance at 82% and 86% for daily and monthly calibration respectively. Although the simulated flow patterns matched the observed flow, the discharge volumes were also analyzed. The Volumetric Efficiency (VE) metric formulated by Criss and Winston [43] serves to evaluate the timing of the flow and ranges from 0 to 1. The VE values indicated that 72% and 75% of the water was delivered at the right time during the daily and monthly calibration, respectively. Compared to the ideal VE value of 1, the values showed that the model satisfactorily simulated discharge volume timing.

4.2 Parameter identification

The identification of the sensitive parameters was analyzed to assess the effectiveness of the algorithm in SWAT model calibration. This was achieved by tracking the evolution and convergence of parameter values, global optimum and the Normalized Swarm Radius (NSR). **Error! Reference source not found.** shows the evolution of parameters CN2,

ESCO, GW_REVAP and CH_K2. The convergence in all the parameters shows a narrow parameter space at 20,000 model evaluations (Fig. 3). This shows that the algorithm

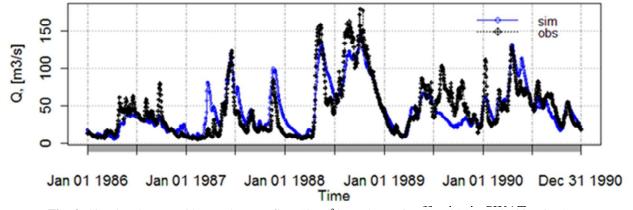


Fig. 2: Simulated versus Observed streamflow (Q, m³/s) at the station 1DD01A (marked in Fig. 1)

As shown in Fig. 2, the simulated flow matched the observed flow well in terms of overall patterns during the calibration period. However, some of the peak flows were not well simulated. The PBias, R² and NSE values for daily simulation reached -1.4, 0.73 and 0.72, respectively, while for monthly calibration these values were -1.4, 0.78 and 0.77 respectively. Given that the NSE values are dependent on the mean flows, the low absolute difference between the mean observed and mean simulated flows (45.23 m³ s⁻¹ and 44.58 m³ s⁻¹ respectively) contributed to the satisfactory NSE values.

model calibration. Frequency histograms of posterior parameter values for eight parameters are shown in Fig. 4. The identification of the parameter showed irregular and skewed distribution shapes which signify great uncertainty on their most probable optimum value. However, the parameters are well defined as the peak of the posterior distribution is sharp around the best value in all parameters expect ALPHA_BF and SOL_AWC. An initial exploration phase occurs in global optimum up to about 100 iterations (Fig. 5). The initial exploration in





NSR occurs up to about 375 iterations. Both the global optimum and the NSR show a clear convergence around the NSE value of 0.67. Interaction between parameters at

different NSE values between the observed and simulated streamflow is highlighted through the 2-dimensional dotty-plots shown in Fig. 6.

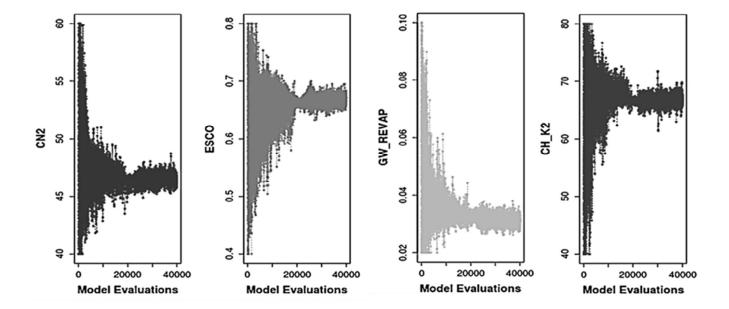


Fig. 3. Parameter value evolution for the 1000 model iterations and 40 swarm particles (making a total of 40,000 model evaluations)





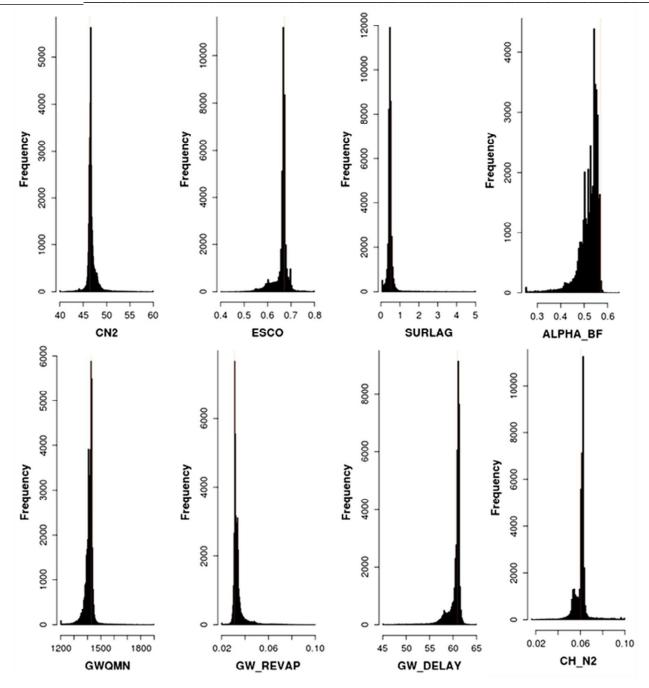


Fig. 4. Frequency histograms for the calibrated parameters (full definitions of the parameters are shown in Table 1)



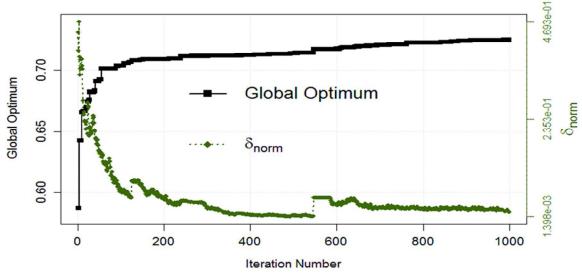


Fig. 5. Evolution of the Global Optimum and the Normalized Swarm Radius (δ_{norm}) over the 1000 model iterations

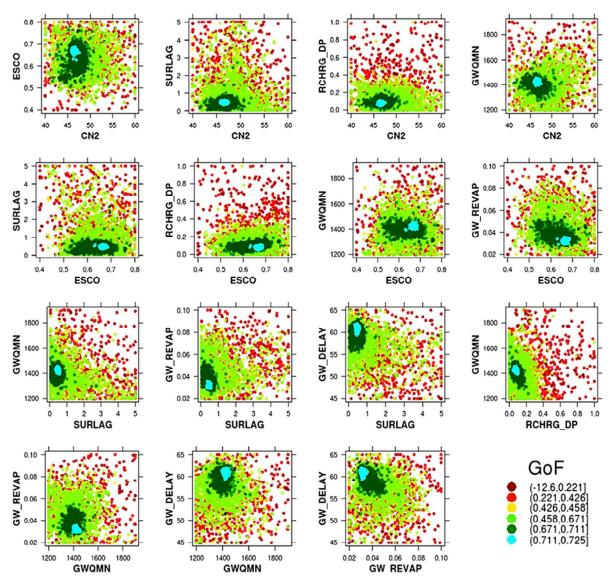


Fig. 6. 2-dimensional dotty-plots showing the interaction between calibration parameters at different NSE values



In the simulation of hydrological process, input data errors, model structure inefficiencies and parameter calibration contribute to overall modeling uncertainties. In this paper, parameter uncertainty was analyzed in terms of a 95% confidence interval (CI) as shown in

Table 2. This was obtained by setting 0.5 as the threshold NSE value and ordering the parameter samples for the behavioral simulations to determine the 2.5% and 97.5% threshold parameter values. A total of 951parameter sets were sampled from the 40 swarms and 1000 iterations. The distribution of parameter values in all sampled parameter sets showed statistically significant deviations from normality. The uncertainty range for CN2 is from 46.4 to 50.4. The base flow recession constant (ALPHA_BF) affects the simulation of groundwater recharge and its uncertainty range varied from 0.46 to

0.57. The uncertainty range for the surface runoff lag coefficient (SURLAG) varied from 0.27 to 0.52.

The 95% CI parameter sets were used to simulate streamflow to determine the extent to which parameter uncertainty contributes to total uncertainties in streamflow modeling in the area (Fig. 7). The 95% CI is shown by grey shading while the solid line shows the observed streamflow. The more observations contained by the CI bracket, the greater the contribution of parameter uncertainty to overall simulation uncertainty. About 35% of the daily stream flow observations fall within the 95% CI (Fig. 7). Therefore, parameter uncertainty can only account for a small portion of the overall simulation uncertainty. In addition, the width of stream flow 95% CI showed a temporal variation corresponding to rainfall amount which emphasizes a high level of uncertainty during the high rainfall season. However, this could also be

Table 2: 95% CI for calibration parameters

| Parameter | 95%CI | Parameter | 95%CI |
|-----------|--------------------|-----------|----------------|
| CN2 | [50.4, 46.4] | ALPHA_BF | [0.46, 0.57] |
| ESCO | [0.76, 0.67] | SOL_K | [35.03, 15.24] |
| SURLAG | [0.27, 0.52] | EPCO | [0.53, 0.43] |
| RCHRG_DP | [0.15, 0.06] | SOL_AWC | [0.25, 0.23] |
| GWQMN | [1317.35, 1431.56] | OV_N | [0.58, 0.59] |
| GW_REVAP | [0.04, 0.03] | CH_N2 | [0.03, 0.06] |
| GW_DELAY | [58.24, 60.99] | CH_K2 | [74.83, 66.91] |



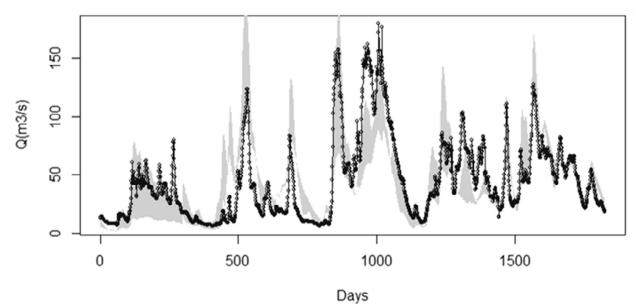


Fig. 7. Simulation uncertainty caused by parameter uncertainty in the 1986 to 1990 period.

attributed to rainfall events covering small spatial extents assumed to cover large areas in the SWAT model.

Fig. 8 shows the Empirical Cumulative Distribution Functions (ECDFs) of the 5, 50 and 95 quantiles and an estimation of the percentage bias for the specified quantiles. The vertical dashed-line represents the observed (black) and simulated (gray) quantiles. Low flows were often overestimated (Bias= 13.8% for the Q5), while the Q50 and Q95 were underestimated with biases of -4.2% and -13.1%, respectively (Fig. 8).

The concept of "equifinality' highlighted by Beven and Binley [13] was also evident in the estimation of optimum parameter values. This is shown in Table 3 whereby different parameter sets yielded the same NSE value hence indicating uncertainty in optimum SWAT parameter values for Nzoia Basin. In previous studies, this has been attributed to multiple factors affecting parameter identifiability during calibration, such as parameter correlations, scale (spatial and temporal) of the simulation, statistical characteristics of model errors, as well as parameter sensitivity or insensitivity [7]. Consequently, the SWAT model parameter identification analysis is recommended under different model conceptualization and temporal scales in the area.

Table 3: The equifinality of model parameters

| ъ. | 0 . 1 | 0 . 0 | g . 2 |
|-----------|---------|---------|---------|
| Parameter | Set 1 | Set 2 | Set 3 |
| CN2 | 56.02 | 47.44 | 50.40 |
| ESCO | 0.56 | 0.57 | 0.76 |
| SURLAG | 0.05 | 0.35 | 0.27 |
| RCHRG_DP | 0.00 | 0.12 | 0.15 |
| GWQMN | 1522.45 | 1362.17 | 1317.35 |
| GW_REVAP | 0.07 | 0.05 | 0.04 |
| GW_DELAY | 54.09 | 58.45 | 58.24 |
| ALPHA_BF | 0.25 | 0.44 | 0.46 |
| SOL_K | 138.26 | 70.61 | 35.03 |
| EPCO | 0.58 | 0.45 | 0.53 |
| SOL_AWC | 0.15 | 0.21 | 0.25 |
| OV_N | 0.56 | 0.55 | 0.58 |
| CH_N2 | 0.04 | 0.09 | 0.03 |
| CH_K2 | 43.38 | 61.00 | 74.83 |
| NSE | 0.67 | 0.67 | 0.67 |





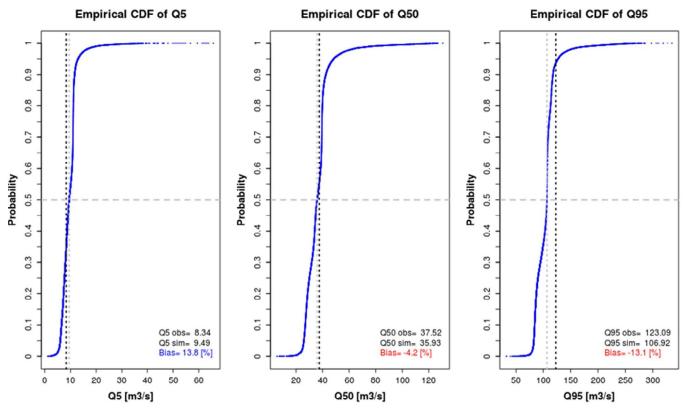


Fig. 8. The Empirical Cumulative Distribution Functions (ECDFs) for 5%, 50% and 95% quantiles.

5. Conclusions

The efficient estimation of optimum parameters values is inevitable in hydrological modeling. In this paper, the HydroPSO R package was applied to SWAT model in R software to assess parameter identification and calibration in Nzoia Basin. Fourteen parameters representing the surface flow, subsurface flow and channel routing components of the water balance were selected for model optimization. The following conclusions can be drawn from the results of the study:

- i. The SWAT model effectively simulated streamflow in the study area considering the three main performance evaluation metrics used. The simulated low flows showed overestimation, while the median and high flows were underestimated. The model parameters were not well identifiable as shown by the skewed posterior distribution of parameter sets. The evolution of parameter values against the model evaluations showed similar convergence for all the 11 calibrated parameters.
- ii. The HydroPSO R package can be successfully combined with the SWAT model in R software to harness the combined benefits of a distributed hydrological model and flexible computing capability of the open source R software.

iii. Parameter uncertainty accounted for about 35% of the overall model uncertainty. However, we acknowledge that model error and input data are also major sources of uncertainty in hydrological modelling. It is therefore recommended that further studies focusing on multi-objective consideration of uncertainty sources in hydrological modelling of the Nzoia Basin be carried out. Coordinated field studies and monitoring can also be conducted to determine important physical parameters for improved watershed management in the area.

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