A Proposed Methodological Framework for the Spatial and temporal Calibration of a Large River Basin Hydrological Model

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Abstract:

Under a whole system scale analysis, hydrological modelling of large river basins is critical to understand the behaviour of regional phenomena and cumulative impacts. Many hydrologic models contain parameters that are difficult to measure or do not have a direct physical interpretation, so it is necessary to estimate these model parameters using a calibration procedure. However, observations for calibration and validation are only available for specific locations and more formal procedures are necessary to regionalize model parameters in areas with limited or without data. In this paper, a methodological framework for the spatial and temporal calibration of a large river basin hydrological model is proposed that uses a cluster method to group sub-catchments of the macro basin model, based on its morphometric characteristics, under the assumption that catchments in the same group share the same parameter values in the model. The methodology was tested in a Magdalena-Cauca (Colombia) macro basin hydrological model

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A Proposed Methodological Framework for The Spatial and Temporal Calibration of a Large River Basin Hydrological Model

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Abstract

Under a whole system scale analysis, hydrological modelling of large river basins is critical to understand the behaviour of regional phenomena and cumulative impacts. Many hydrologic models contain parameters that are difficult to measure or do not have a direct physical interpretation, so it is necessary to estimate these model parameters using a calibration procedure. However, observations for calibration and validation are only available for specific locations and more formal procedures are necessary to regionalize model parameters in areas with limited or without data. In this paper, a methodological framework for the spatial and temporal calibration of a large river basin hydrological model is proposed that uses a cluster method to group sub-catchments of the macro basin model, based on its morphometric characteristics, under the assumption that catchments in the same group share the same parameter values in the model. The methodology was tested in a Magdalena-Cauca (Colombia) macro basin hydrological model developed in the Water Evaluation and Planning (WEAP) software (Stockholm Environmental Institute, Stockholm, Sweden). The results show a Nash-Sutcliffe efficiency coefficient between 0.45 and 0.83 in calibration and between 0.43 and 0.83 in validation.

Keywords: Large river basin, Hydrological models, Calibration, Cluster method.

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1. Introduction

Studies aimed to understand the hydrological response at the system level imply a significant change in the scale of analysis with a broader comprehension of the phenomena and events that occur in the basin. Hydrological modelling is presented as a tool of great importance in this type of analysis for the comprehension of the integral behaviour of the macro basin.

As pointed out by Wagener *et al.* (2001), most hydrological models are classified as conceptual. This implies that the model parameters often do not have a direct physical interpretation and therefore cannot be measured in the field. For some other models, it is possible that their parameters have physical interpretation, however, for many cases, there is no data measured in the field that allows their calculation. Therefore, for most hydrological model structures currently used, the model parameters must be estimated using a calibration procedure that allows to have a set of parameters that brings an acceptable level of agreement between the measured system output and the model response (Wagener *et al.*, 2001).

For hydrological models in large river basins, observations for calibration and validation of the model are often only available at a subset of sites where the model is applied. For sites without observations, the parameters must be determined based on global parameters (Engeland *et al.*, 2001). The model can be calibrated on some of the available data and then validated on data from period of times not used (Klemes, 1986). As the parameters can be regionalised to relate them to catchment characteristics (Johansson, 1994), a second validation can be performed on data that is available in catchments in the same region, but not used in the calibration.

The previous procedure presents big challenges in terms of the calibration of a macro basin model, including best practices for regionalization of the units of the model and a clearer way to transfer the calibrated parameters in specific sites of the model to other sites that

were not used in the calibration process. This paper proposes a methodological framework for the calibration of a large river basin hydrological model that allows the identification of similar units (sub-catchments) in the macro model, in which each group of these similar units share like-parameter values. The methodology also uses objective calibration methods and the Generalised Likelihood Uncertainty Estimation (GLUE) method (Beven and Binley, 1992).

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2. Proposed Methodological Framework

The proposed methodological procedure is summarized in Figure 1.

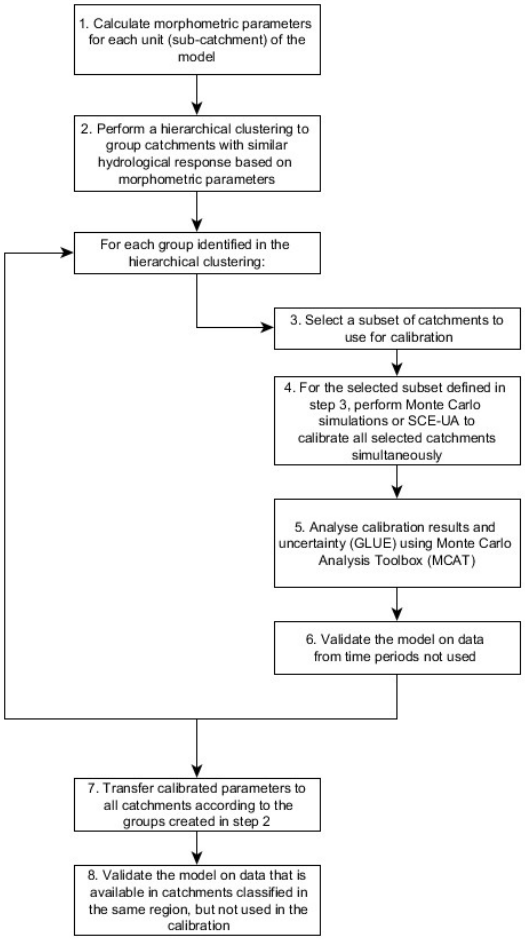

Figure 1. Proposed methodological procedure for calibration of large river basin hydrological models

As shown above, the methodology consists of 8 main steps that are described as follows:

1. *Calculate morphometric parameters*

The first step in the proposed procedure is to calculate a set of morphometric parameters for each sub-catchment in the model. To have an extensive characterization of the units of the model, we recommend at least the calculation of the 28 morphometric variables that are presented in Table 1, described as Faris (2015).

Table 1. Description of morphometric parameters proposed for the sub-catchment characterization (Adapted from Faris, 2015)

ID	Morphometric Parameter	Formula	Author
1	Total basin area (A) (Km^2)	Projected area enclosed by basin boundary	Schumm (1956)
2	Total basin perimeter (P) (Km)	Length of horizontal projection of basin water divide	Schumm (1956)
3	Basin length (Lb) (Km)	Distance from outlet to farthest point on basin boundary	Schumm (1956)
4	Fitness ratio (Rf)	$Rf = \frac{Lb}{P}$	Melton (1957)
5	Form factor (Ff)	$Ff = \frac{A}{Lb^2}$	Horton (1932)
6	Shape factor (Sf)	$Sf = \frac{Lb^2}{A} = \frac{1}{Ff}$	Strahler (1957)
7	Relative perimeter (Rp)	$Rp = \frac{A}{P}$	Schumm (1956)
8	Length area relation (Lar)	$Lar = 1.4A^{0.6}$	Hack (1957)

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ID	Morphometric Parameter	Formula	Author
9	Rotundity coefficient (Rc)	$Rc = \frac{Lb^2\pi}{4A}$	Strahler (1957)
10	Mean basin width (Wb)	$Wb = \frac{A}{Lb}$	Horton (1932)
11	Drainage texture (Dt)	$Dt = \frac{Number\ of\ stream\ orders\ (Nu)}{P}$	Horton (1945)
12	Compactness coefficient (Cc)	$Cc = \frac{0.282P}{\sqrt{A}}$	Horton (1945)
13	Circularity ratio (Cr)	$Cr = \frac{4\pi A}{P^2}$	Miller (1953)
14	Elongation ratio (Re)	$Re = \frac{1.129\sqrt{A}}{Lb}$	Schumm (1956)
15	Drainage density (Dd)(Km/Km^2)	$Dd = \sum_{i=1}^{k}\sum_{i=0}^{N} \frac{Length\ of\ stream\ orders\ (Lu)}{A}$	Strahler (1957)
16	Stream frequency (F) (number/km^2)	$F = \sum_{i=1}^{k} \frac{Nu}{A}$	Horton (1932)
17	Constant of channel maintenance (Ccm) (km^2/km)	$Ccm = \frac{1}{Dd} = \frac{A}{\sum_{i=1}^{k}\sum_{i=0}^{N}\frac{Lu}{A}}$	Schumm (1956)
18	Infiltration number (Ifn)	$Ifn = FxDd$	Farinan (1952)
19	Drainage intensity (Di)	$Di = \frac{F}{Dd}$	Farinan (1952)
20	Average length of overland flow (Lg) (Km)	$Lg = \frac{1}{2Dd}$	Horton (1945)
21	Height of basin outlet (z) (m)	Selected point elevation from DEM	

ID	Morphometric Parameter	Formula	Author
22	Maximum height of basin (Z) (m)	Selected point elevation from DEM	
23	Total basin relief (H)	$H = Z - z$	Strahler (1952)
24	Relief ratio (Rhl)	$Rhl = \frac{H}{Lb}$	Schumm (1956)
25	Relative relief ratio (Rhp)	$Rhp = \frac{(H)(100)}{P}$	Melton (1957)
26	Gradient ratio (Rg)	$Rg = \frac{Z - z}{Lb}$	Sreedevi *el al.* (2005)
27	Ruggedness Number (Rn)	$Rn = Dd\frac{H}{1000}$	Strahler (1952)
28	Melton ruggedness number (MRn)	$MRn = \frac{H}{\sqrt{A}}$	Melton (1965)

For the calculation of the morphometric parameters, the morphometric toolbox developed by Faris (2015) can be used in batch mode to obtain the characterization for all sub-catchments of the model.

2. Hierarchical clustering

In the second step of the methodology, the main objective is to group sub-catchments of the model based on the similarity of their morphometric parameters. For this, the use of agglomerative hierarchical clustering is proposed.

As described by Jain and Dubes (1988), a hierarchical clustering method is a procedure for transforming a proximity matrix into a sequence of nested partitions. In the agglomerative

hierarchical approach, each data point starts as a cluster and, at each step, existing clusters are combined. There are different methods for this, including single linkage, complete linkage, average linkage and centroid method, among others. There is no a correct method or best method for the analysis. In practice, it is advisable to compare the results of several methods to take a final decision about the formation of clusters.

The hierarchical cluster analysis can be performed using the cluster package (Maechler *et al.,* 2018) in R (R Core Team, 2018). As presented in R documentation, initially this function assigns each object to its own cluster and then the algorithm proceeds iteratively, at each stage joining the two most similar clusters, continuing until there is just a single cluster (R Core Team, 2008). At each stage, distances between clusters are recomputed by the Lance-Williams dissimilarity update formula according to the particular clustering method being used (R Core Team, 2008).

The R function can analyse the data using different clustering methods, including those that are mentioned before. Table 2 presents the mathematical expressions for the main methods that can be used for the hierarchical clustering. Based on the definition of the distance between clusters, at each stage of the process the two clusters that have the smallest distance are combined.

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Table 2. Mathematical expressions and descriptions of the main methods for the hierarchical clustering (Adapted from Pennsylvania State University, 2017)

Method	Definition of distance between two clusters	Mathematical Expression
Single Linkage	Minimum distance between any single data point in the first cluster and any single data point in the second cluster.	$d_{12} = \min_{ij} d(x_i, y_j)$
Complete Linkage	Maximum distance between any single data point in the first cluster and any single data point in the second cluster.	$d_{12} = \max_{ij} d(x_i, y_j)$
Average Linkage	Average distance between data points in the first cluster and data points in the second cluster	$d_{12} = \frac{1}{kl}\sum_{i=1}^{k}\sum_{j=1}^{l} d(x_i, y_j)$
Centroid Method	Distance between the two mean vectors of the cluster	$d_{12} = d(\bar{x},\bar{y})$

To facilitate the interpretation of the hierarchical clustering results, a dendrogram is an especially useful scheme. A dendrogram is a type of tree structure that provides a much easier way to understand the clustering exercise. It consists of layers of nodes, each representing a cluster. Lines connect nodes representing clusters which are nested into one another (Jain and Dubes, 1988). Figure 2 presents an example of dendrogram.

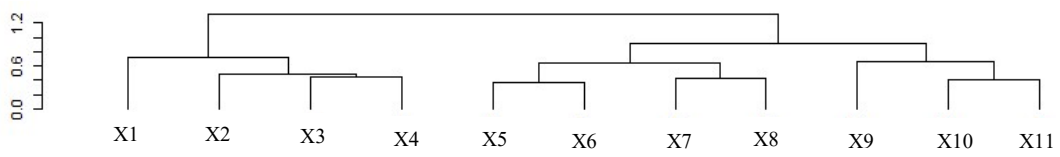

Figure 2. Example of dendrogram

The objective of this procedure is to identify units of the model (sub-catchments) that share parameters, under the assumption that units that are grouped in the same cluster, based on the analysis of its morphometric parameters, also have similar hydrological parameters in the model. Thus, the most important aspect of this second step in the methodology is to decide the way the groups will be finally created. As cutting a dendrogram horizontally at any level defines a clustering and identifies clusters (Jain and Dubes, 1988), it will be enough to define a cut level of the dendrogram to establish the sub-catchments of the model that will belong to the same cluster. The level itself has no meaning in terms of the scale of the proximity matrix (Jain and Dubes, 1988), so the modeler has the responsibility to define the cut level based on the availability of data and the heterogeneity of the system modelled.

After this procedure, there will be *n* clusters composed of *m* sub-catchments. The sub-catchments in a particular group, at first, share the same hydrological parameters in the model. The modeler must verify that in each cluster, at least one unit of the model (sub-catchment) has data for calibration and validation. If there are clusters without any sub-catchment with data for calibration, these clusters must be grouped with the nearest cluster with data to create a calibration group. It is important to recognize that for that clusters that must be grouped with other clusters due to lack of information, the uncertainty is higher.

3. *Select a subset of catchments for calibration and validation*

For each cluster identified in step 2, a subset of units of the model (sub-catchments) for calibration must be selected. Ideally, each model will have multiple sub-catchments with data suitable for both spatial and temporal calibration and validation so that calibration and validation are possible. However, this is not always the case.

For those groups with only one sub-catchment with data available for calibration, only temporal calibration and validation is possible. In these cases, the validation will be only on

data from period of times not used (Klemes, 1986), so greater uncertainty of the model response is expected.

In other cases, there will be more than one sub-catchment in the group with data suitable for spatial and temporal calibration. A decision about what sub-catchments are going to be used for spatial calibration, and what sub-catchments will be used for validation must be made. As a recommendation in the methodological procedure, three main aspects to filter out sub-catchments for calibration should be considered:

- Data series length: Usually, the length of the available data in each sub-catchment is different. It is recommended to prioritize sub-catchments with longer data series for calibration.
- Data series quality: It is essential to consider the quality of the available data. In many cases, even though a long set of data is available for calibration, due to problems in the measurement procedures or the instrumentation, some of the data are not good for calibration. Prior analysis about the quality of the data must be done for the selection of the units of the model that are going to be used in the calibration process. The sub-catchments with the best data quality should be consider as best candidates for the calibration procedure.
- Computational time of the model: This criterion will establish the maximum number of sub-catchments that can be considered for simultaneous calibration of each group. The computational time for big macro basin models can be considerable and limit options for calibration of the mathematical model. The final selection of the number of sub-catchments in each group that will be used in the simultaneous calibration procedure should be a balance between the computational available resources, in terms of computational time and capacity, and the desirable average representativeness of the parameters for all the units of the model that are part of the same group.

At the end of this step, a subset of sub-catchments for spatial calibration are selected. It is important to notice that with the selection of the sub-catchments for calibration, the sub-catchments for spatial validation will be automatically selected. Sub-catchments for spatial validation are the sub-catchments that were considered through the aspects described in the three main criteria for filtering, but were not selected at the end for calibration, due to restrictions related with data series length or computational time, but that also fulfill the requirements in data quality.

4. Objective calibration

Once the sub-catchments for calibration have been selected, the calibration procedure can be performed. For calibration, the use of automatic search algorithms is recommended to overcome the time-consuming procedure of manual calibration (Wagener *et al.*, 2001). Traditionally, in the calibration stage, the parameters are estimated using a procedure whereby they are adjusted until the model output and the measured historical data show an acceptable level of agreement. To measure the agreement, usually an objective function is used (Wagener *et al.*, 2001). However, one of the most important limitations in a classical approach to model calibration is the impossibility to find a unique best parameter set that obviates other feasible parameter sets (Gupta *et al.*, 1998). To address this problem, a multi-objective view is proposed by Gupta *et al.* (1998) and it is recommended as a good way to understand the complexity of a macro basin model.

In regard to automatic search algorithms, Monte Carlo simulations or population-evolution-based search strategies are good options for the procedure. Particularly, Duan *et al.* (1992) has demonstrated that the population-evolution-based Shuffled Complex Evolution (SCE-UA) global optimization algorithm is a consistent, effective and efficient method in locating the globally optimal model parameters of a hydrological model (Duan *et al.*, 1992;

Sorooshian *et al.*, 1993; Luce and Cundy, 1994; Gan and Biftu, 1996; Tanakamaru, 1995; Tanakamaru and Burges, 1997; Kuczera, 1997).

The use of Monte Carlo simulations or SCE-UA depends on the complexity of the model and again on the computational time of the model. For a complex model, a large number of Monte Carlo simulations may be needed to explore in an extensive way the entire parametric space. In this case, the use of the SCE-UA method is better.

For each group identified in step 2, there are a set of selected sub-catchments for calibration, so we propose using a simultaneous calibration procedure in which the values of the objective functions used to evaluate the adjustment of the model in each clustered group are calculated simultaneously. This strategy generates a large amount of information suitable for analysis to define the better parameters to use in the model.

The SCE-UA algorithm uses an objective function that must be minimized, so we propose the use of an average traditional objective function for this purpose. For example, the average of the Nash-Sutcliffe (NSE) efficiency coefficient can be calculated as the summation of the individual Nash-Sutcliffe of each sub-catchment selected for calibration (evaluated for the same set of parameters) divided by the number of sub-catchments involve in the procedure:

$$\overline{NSE} = \frac{\sum_{i=1}^{n} NSE_i}{n} \quad (1)$$

It must be noted that because the NSE varies between 1 (most desirable) and -∞ and the SCE-UA algorithm minimizes the objective function, 1-$\overline{NSE}$ must be used so that the most desirable value would be 0.

It is important to mention that is highly recommended to calculate different objective functions in the calibration procedure to have a multi-objective view of the problem and to have enough data to study the equifinality problem (Beven and Binley, 1992). Some of the

objective functions that can be used in the analysis are presented in Table 3 (d_o is the observed data and d_m is the modelled data).

Table 3. Examples of objective functions that can be used as part of the analysis

Notation	Objective Function	Equation
NSE	Nash-Sutcliffe Efficiency	$1-\frac{\sum(d_o-d_m)^2}{\sum(d_o-\overline{d_o})^2}$
APBIAS	Absolute Percent Bias	$\frac{\sum\lvert d_o-d_m\rvert}{\sum d_o}*100$
RBIAS	Relative Percent Bias	$\left(\frac{\frac{1}{n}\sum(d_m)}{\frac{1}{n}\sum(d_o)}-1\right)$*100
RMSE	Root Mean Square Error	$\sqrt{\frac{1}{n}\sum(d_o-d_m)^2}$
ABSERR	Mean Absolute Error	$\frac{1}{n}\sum\lvert d_o-d_m\rvert$

Another aspect that must be considered is that a period of time for calibration must be selected. It is recommended that the period should be common between all the sub-catchments selected for calibration in each group so the simulation in the model will be made for the same period for the calibration procedure. The period of time left, not used for calibration, will be used for a first validation exercise.

5. *Analyse calibration results and model parameter uncertainty*

A deep analysis of the calibration and the estimation of uncertainty of the model parameters are indispensable procedures in the proposed methodological framework. A holistic model evaluation in this stage includes the detailed investigation of model performance, model structure suitability, parameter identifiability and prediction

uncertainty. All these analysis helps to understand the behaviour of the model and its performance, recognizing also its limitations and reliability of the results (Wagener *et al.,* 2001).

The Monte Carlo Analysis Toolbox (MCAT; Wagener *et al.,* 1999) is a collection of Matlab (Mathworks, 2017) analysis and visualisation functions integrated through a graphical user interface (Wagener *et al.,* 2001a). The toolbox can be used to analyse the results from Monte Carlo simulations or from model optimisation methods that are based on population evolution techniques (e.g. SCE-UA) (Wagener *et al.*, 1999). MCAT includes several functions like Regional Sensitivity Analysis (Spear and Homberger, 1980), Generalised Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992), multi-objective analysis (Gupta *et al.*, 1998) and different kinds of plots to analyse parameter identifiability and interaction (Wagener *et al*., 2001a).

Specifically, as described by Wagener *et al.* (2001a), the system architecture of the Monte Carlo Analysis Toolbox comprises:

- Class plots
- Dotty plots
- 2-D and 3-D surface plots
- Dynamic identifiability analysis
- GLUE Regional sensitivity analysis
- GLUE Confidence limits
- GLUE variable uncertainty
- A posteriori parameter distributions
- Multi-Objective (MO) Analysis
- Multi-Objective (MO) Parameter Rankings
- Multi-Objective (MO) Pareto Confidence Limits
- Multi-Objective (MO) Normalized Parameter ranges

A complete discussion about the functionalities of MCAT is presented by Wagener *et al.* (2001a). The use of the MCAT is recommended in the methodological procedure for the calibration of large river basin hydrological models due to its recognized utility in the analysis of model calibration and structure.

The analysis with MCAT of the Monte Carlo experiments or the population-evolution-based results determines the best set of parameters. Thus, for each group defined for the model, there will be a selected set of parameters that will characterize the entire region based on a simultaneous calibration procedure and an integral analysis of the results with model parameter uncertainty estimation.

6. Temporal calibration and validation

Following Klemes (1986), the split-sample test technique is recommended for this step in which the available record for each sub-catchment selected for spatial calibration is been split into two segments (periods), one of which has been used for calibration, and the second period is used for validation.

If the available record is sufficiently long so that one half of it is suitable for calibration, it should be split into two equal parts, each of them should be used for calibration and validation (Klemes, 1986). In the case that the available data is not long enough for a half splitting, the record should be split in a way that the calibration period is long enough for a meaningful calibration and the reminder serving for validation (Klemes, 1986).

The model should be judged acceptable only if the calibration and validation results are acceptable (Klemes, 1986).

7. *Transfer calibrated parameters to sub-catchments in the defined groups*

If the results in step 6 are acceptable, meaning that the calibration and validation results were satisfactory, the next step is to apply the selected parameters for each group to the other sub-catchments that are part of the same cluster, as defined in step 2, but that were not used for the calibration procedure, either because there are no data available in the sub-catchment for calibration or because the sub-catchment was selected for the second validation following criteria proposed in step 3.

At the end of this step, all sub-catchments in the model must have calibrated parameters according to their respective clusters.

8. *Validate on data that is available in sub-catchments not used in the calibration*

A final validation of the model must be done in sub-catchments with available data but that were not selected for the calibration procedure. In all basins that have measured data, a simulation with the calibrated parameters that were assigned in step 7 must be performed and the results must be evaluated to establish its acceptability.

3. Results and discussion

The proposed calibration methodology was tested in a model for the Magdalena-Cauca macro basin in Colombia, developed in WEAP (Water Evaluation and Planning) (Stockholm Environmental Institute, Stockholm, Sweden). The characteristics of the model are summarised in Table 4.

Table 4. Description of the WEAP Magdalena-Cauca Model

Characteristic	Description
Modelling Software	Water Evaluation and Planning (WEAP) (SEI, 2016).
Modelling Domain	Magdalena-Cauca rivers represented as 391 hydrological units
Hydrological Model	Soil Moisture Model
River Units	194
Diversions	19
Large Scale Infrastructure	Hydropower development scenarios: A. Baseline 2016: 33 projects B. Full development portfolio: 128 projects (120 reservoirs and 8 run-of-river)
Aquifer System	24 main units identified in underground water map of Colombia.
Resolution and temporal extent	Monthly, 30 years of simulation

The model was calibrated and validated according to the proposed methodological framework (section 2). A brief description of the procedure and the main results are described below.

1. *Calculate morphometric parameters*

All 391 hydrological units (sub-catchments) of the model were characterized by the 28 morphometric parameters described in Table 1, using the morphometric toolbox for ArcGIS (Faris, 2015). The range of values obtained in the analysis are presented in

Table 5.

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Table 5. Results for morphometric characterization of the units of the WEAP Magdalena-Cauca Model

ID	Morphometric Parameter	Higher Value	Lower Value
1	Total basin area (A) (Km^2)	7938.01	20.28
2	Total basin perimeter (P) (Km)	500.41	19.58
3	Basin length (Lb) (Km)	164.55	8.67
4	Fitness ratio (Rf)	1.57	0.12
5	Form factor (Ff)	1.22	0.02
6	Shape factor (Sf)	51.32	0.82
7	Relative perimeter (Rp)	17.28	1.04
8	Length area relation (Lar)	303.84	8.52
9	Rotundity coefficient (Rc)	40.31	0.65
10	Mean basin width (Wb)	75.41	1.53
11	Drainage texture (Dt)	1.33	0.04
12	Compactness coefficient (Cc)	2.63	1.16
13	Circularity ratio (Cr)	0.74	0.14
14	Elongation ratio (Re)	1.25	0.16
15	Drainage density (Dd)(Km/Km^2)	0.91	0.17
16	Stream frequency (F) ($number/km^2$)	0.14	0.02
17	Constant of channel maintenance (Ccm) (km^2/km)	6.04	1.10
18	Infiltration number (Ifn)	0.10	0.01
19	Drainage intensity (Di)	0.51	0.05
20	Average length of overland flow (Lg) (Km)	3.03	0.55
21	Height of basin outlet (z) (m)	3076	-34
22	Maximum height of basin (Z) (m)	5543	14
23	Total basin relief (H)	5530	39
24	Relief ratio (Rhl)	0.16	0.00
25	Relative relief ratio (Rhp)	6.38	0.02
26	Gradient ratio (Rg)	0.16	0.00
27	Ruggedness Number (Rn)	0.18	0.01
28	Melton ruggedness number (MRn)	0.29	0.00

As shown above, there is a wide range of variability of the morphometric parameters among the different sub-catchments defined in the model.

2. Hierarchical clustering

First, the values presented in

Table 5 were normalized to vary between 0 and 1. With the normalized values, a hierarchical clustering using the complete linkage method was performed following the procedure described in section 2.

The resulting dendrogram of the analysis includes all 391 elements and is very extensive. As an example, Figure 3 presents a part of the dendrogram corresponding to branch 13 with cut level at 1.

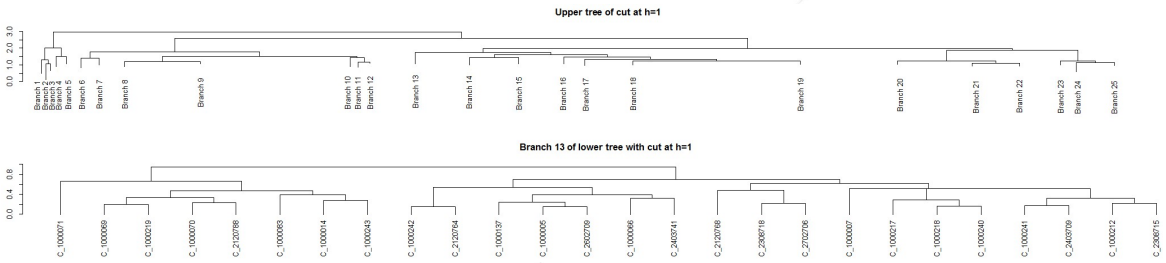

Figure 3. Branch 13 of the dendrogram for the units of the WEAP Magdalena-Cauca model

As shown above, with a cut level of 1.0, 25 clusters were identified. However, there is no data for calibration for all these clusters and therefore a grouping procedure based on the nearest cluster with data was performed. Branches 2, 3, 4, 5, 11, 14, 16, 17, 21 and 22 are the ones without data for calibration. These branches were grouped as shown in Table 6 to configure the final groups for the calibration procedure.

Table 6. Final groups for calibration

Cluster for Calibration	Branches	Number of Sub-Catchments with Data suitable for Calibration in the Cluster
1	1, 2, 3, 4, 5	1
2	6	1
3	7	1
4	8	6
5	9	6
6	10	1
7	11, 12	1
8	13	1
9	14, 15	1
10	16, 17, 18	3
11	19	1
12	20, 21, 22	1
13	23	1
14	24	1
15	25	1

Based on this analysis, a higher uncertainty for the sub-catchments that are part of the calibration clusters 1, 7, 9, 10 and 12, is recognized because they only have one sub-catchment with data suitable for calibration. Figure 4 shows the defined clusters.

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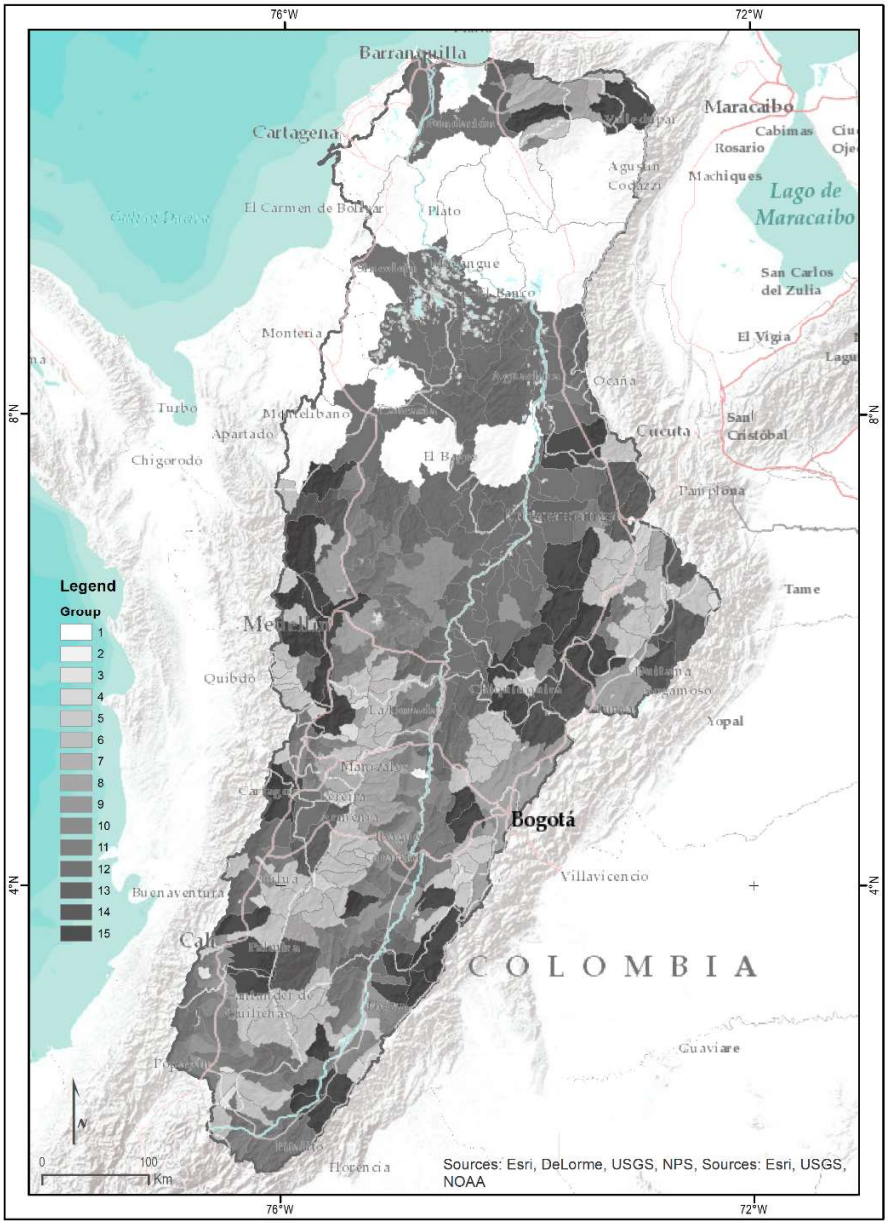

Figure 4. 15 defined clusters for the WEAP Magdalena-Cauca model

3. Select a subset of catchments for calibration

According to the results presented in Table 6, 12 of the 15 clusters in the WEAP Magdalena-Cauca model have only one sub-catchment with suitable data for calibration, so the sub-catchment with data in those 12 clusters was selected for calibration. For the other 3 clusters, a criterion was established to determine how many sub-catchments will be used for the simultaneous calibration and how many will be used for spatial validation.

First, it is important to clarify that the available data was carefully examined to determine if its length and quality fulfil the minimum requirements to be useful for calibration purposes. At least, 20 years of data should be available and the quality of available data was evaluated by comparing precipitation data and the measured flow data.

Taking into account the computational time of the model, a maximum of 3 sub-catchments to calibrate simultaneously was adopted. In the cases that the group has 2 or 3 sub-catchments with adequate data, it was preferred to use these sub-catchments in the simultaneous calibration process instead of leaving sub-catchments for spatial validation.

Table 7 presents a summary of the selection of the sub-catchments for the calibration process. It is important to highlight that clusters identified in Table 7 with no additional sub-catchments for validation are only validated temporally using the data for the period of time that were not used in the calibration using a split sample technique (Klemes, 1986).

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Table 7. Selection of sub-catchments for the calibration process

Cluster	Number of sub-catchments for Calibration	ID of the catchments for Calibration	Number of additional sub-catchments for Validation	ID of the catchments for Validation
1	1	C_2501701	0	-
2	1	C_2605703	0	-
3	1	C_2601704	0	-
4	3	C_2614713 C_2402706 C_2801708	3	C_2118702 C_2609704 C_2617701
5	3	C_2121712 C_2610713 C_2615710	3	C_2613711 C_2306708 C_2206702
6	1	C_2801711	0	-
7	1	C_2615702	0	-
8	1	C_2403741	0	-
9	1	C_2614704	0	-
10	3	C_2402704 C_2602721 C_2602725	0	-

11	1	C_2614704	0	-
12	1	C_2307702	0	-
13	1	C_2612701	0	-
14	1	C_2401759	0	-
15	1	C_2314704	0	-

4. Objective calibration

The calibration procedure was performed for the catchments presented in Table 7 for the period between 1995 and 2004 (10 Years). The SCE-UA method (Duan *et al*, 1992) was used for the calibration based on the code developed for Matlab (Mathworks, 2017). The objective function for the SCE-UA used the average Nash-Sutcliffe efficiency coefficient (1-$\overline{NSE}$), but Root Mean Squared Error (RMSE) and maximum Relative Percent Bias (RBias) were also calculated to be later analysed with MCAT (Wagener *et al.,* 1999).

The parameters of the WEAP Magdalena-Cauca model that were calibrated are described below:

- Albedo (%): Fraction of solar radiation striking a land class that is reflected.
- Cloudiness Fraction (%): Fraction of daytime hours with no clouds.
- Preferred Flow Direction (*f*) (unitless): Used to partition the flow out of the root zone layer between interflow and flow to the lower soil layer or groundwater.
- Deep Conductivity (K_{Deep}) (mm/month): Conductivity rate of the deep layer at full saturation which controls transmission of baseflow.

- Root Zone Conductivity (K_{Root}) (mm/month): Root zone conductivity rate at full saturation which will be partitioned, according to Preferred Flow Direction, between interflow and flow to the lower soil layer.
- Runoff Resistance Factor (*RRF*) (unitless): Used to control surface runoff response. Related to factors such as leaf area index and land slope.
- Soil Water Capacity (*Z1*) (mm): Effective water holding capacity of upper soil layer.
- Initial Z1 (*Z1_Ini*) (%): Initial value of *Z1* at the beginning of a simulation. Relative storage given as a percentage of the total effective storage of the root zone water capacity.
- Deep Water Capacity (*Z2*) (mm): Effective water holding capacity of lower soil layer.
- Initial Z2 (*Z2_Ini*) (%): Initial value of *Z2* at the beginning of a simulation. Relative storage given as a percentage of the total effective storage of the deep water capacity.

The best sets of parameters, based on the average Nash-Sutcliffe efficiency coefficient in each group, are presented in Table 8.

Table 8. Best set of parameters for each group, based on the average Nash-Sutcliffe efficiency

Group	Albedo (%)	Cloudiness Fraction (%)	*f*	K_{Deep} (mm/month)	K_{Root} (mm/month)	*RRF*	*Z1* (mm)	*Z1_Ini* (%)	*Z2* (mm)	*Z2_Ini* (%)
1	22.0	1.6	0.65	473.1	360.1	0.9	307.2	19.9	66.4	31.4
2	21.0	6.0	0.93	494.9	139.5	0.4	293.5	30.0	47.0	35.0
3	22.0	97.0	0.91	346.9	361.7	8.2	239.9	30.0	412.8	35.0
4	20.0	6.6	0.69	327.5	332.9	7.4	241.0	53.0	129.3	40.0
5	17.3	91.6	0.70	77.2	132.8	10.4	439.5	48.4	334.7	44.2
6	20.0	90.0	0.31	304.3	93.5	11.3	259.9	30.0	484.0	35.0
7	17.0	15.0	0.19	233.7	74.0	4.3	352.4	30.0	133.8	35.0
8	22.0	97.0	0.67	99.6	30.0	16.3	312.9	30.0	135.1	35.0
9	20.7	0.8	0.30	80.2	392.2	3.2	70.3	58.5	318.7	33.8
10	16.8	97.6	0.41	200.5	90.1	18.4	420.0	55.1	250.8	39.5

Group	Albedo (%)	Cloudiness Fraction (%)	f	K_{Deep} (mm/month)	K_{Root} (mm/month)	RRF	$Z1$ (mm)	$Z1\_Ini$ (%)	$Z2$ (mm)	$Z2\_Ini$ (%)
11	21.6	10.2	0.62	291.8	293.9	4.0	318.2	47.6	120.4	28.2
12	20.5	4.8	0.73	348.0	476.1	10.8	340.2	59.5	329.8	33.3
13	20.0	15.0	0.14	467.5	147.4	10.7	491.0	30.0	92.62	35.0
14	21.0	66.0	0.90	24.1	87.9	1.7	259.3	30.0	21.9	35.0
15	20.0	20.0	0.70	277.8	101.9	19.0	189.91	30.0	350.4	35.0

The results of the calculated objective functions in the calibration, for the sets of parameters shown in Table 8, are presented in Table 9.

Table 9. Calculated objective functions in calibration

Group	$\overline{NSE}$	$\overline{RMSE}$	$RBIAS_{max}$
1	0.72	602.7	-4.6%
2	0.60	505.3	-4.3%
3	0.67	437.6	-0.1%
4	0.65	319.5	26.2%
5	0.69	146.8	3.7%
6	0.45	268.9	7.7%
7	0.71	336.0	1.6%
8	0.65	63.7	9.3%
9	0.59	279.9	-11.4%
10	0.69	290.1	23.2%
11	0.83	226.0	-1.6%
12	0.72	388.6	-0.1%
13	0.61	425.4	-2.7%
14	0.70	183.2	-1.2%
15	0.59	500.0	-0.8%

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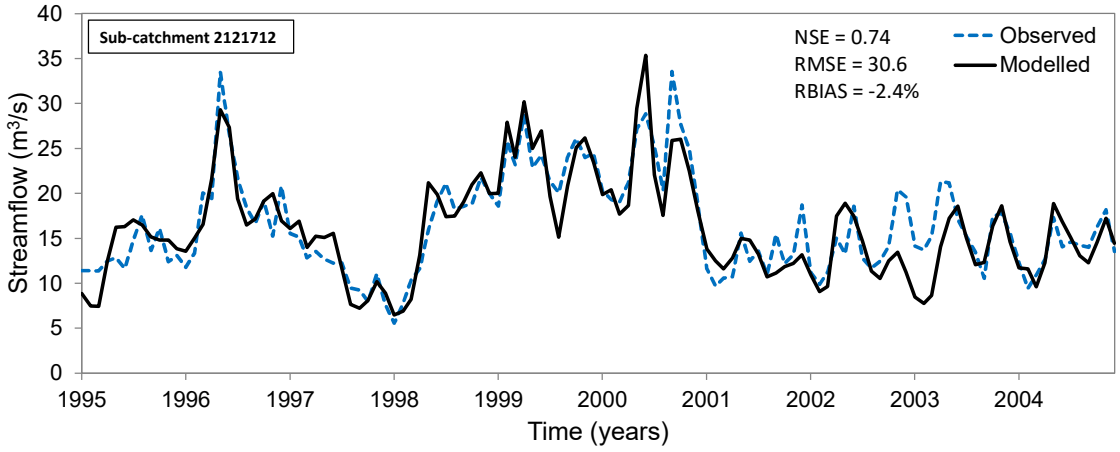
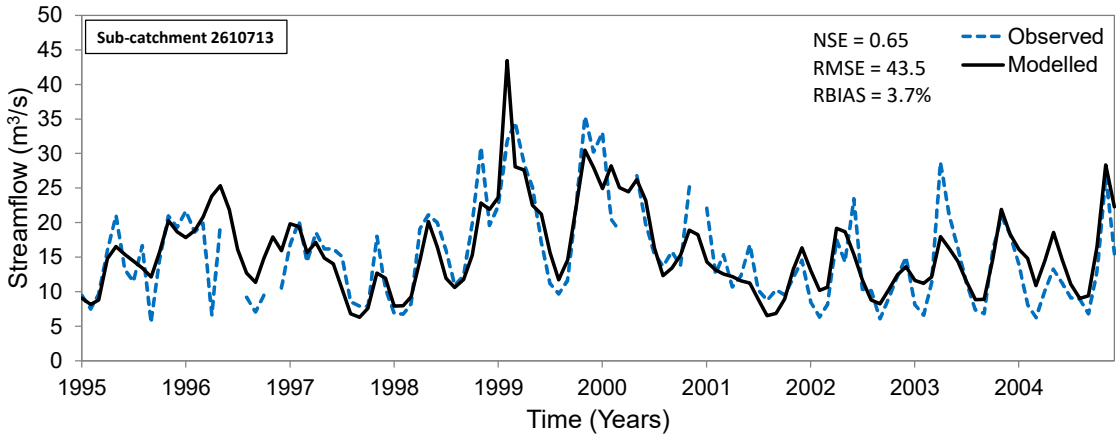
As an example of the calibration results, Figure 5 presents the comparison between the observed streamflow and modelled streamflow for the sub-catchments selected for calibration in cluster 5.





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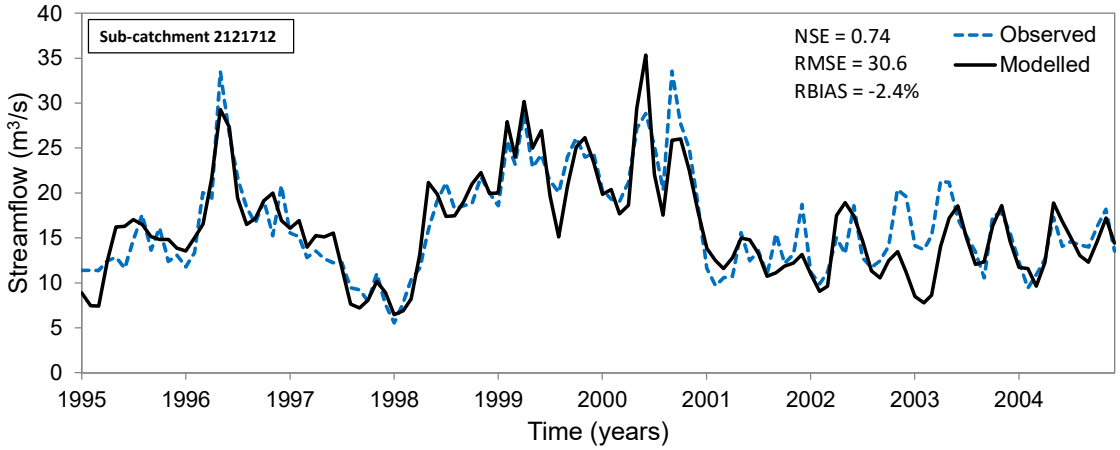

Figure 5. Comparison between observed streamflow and modelled streamflow for calibration for sub-catchments in cluster 5

5. *Analyse calibration results and parameter uncertainty*

For the analysis of the calibration results, the MCAT (Wagener *et al*., 2001a) was used. As the results obtained in the analysis are very extensive, the graphs and outputs of MCAT are focused on the calibration of group 5 as an example of the kind of analysis that are recommended in the methodological framework.

Figure 6 presents the results in dotty plots. Dotty plots represent a projection for the parameter space into 1 dimension. Each dot represents the objective of variable value associated with a single parameter set. If the surface of the dotty plot has a clearly defined minimum, the parameter can be considered to be well identified (Wagener *et al*., 2001a). In this case, all parameters of the model are identifiable, which means that the structure of the Soil Moisture Model is well parametrized. The red dots on the plots identify the optimum set of parameters obtained in the calibration procedure.

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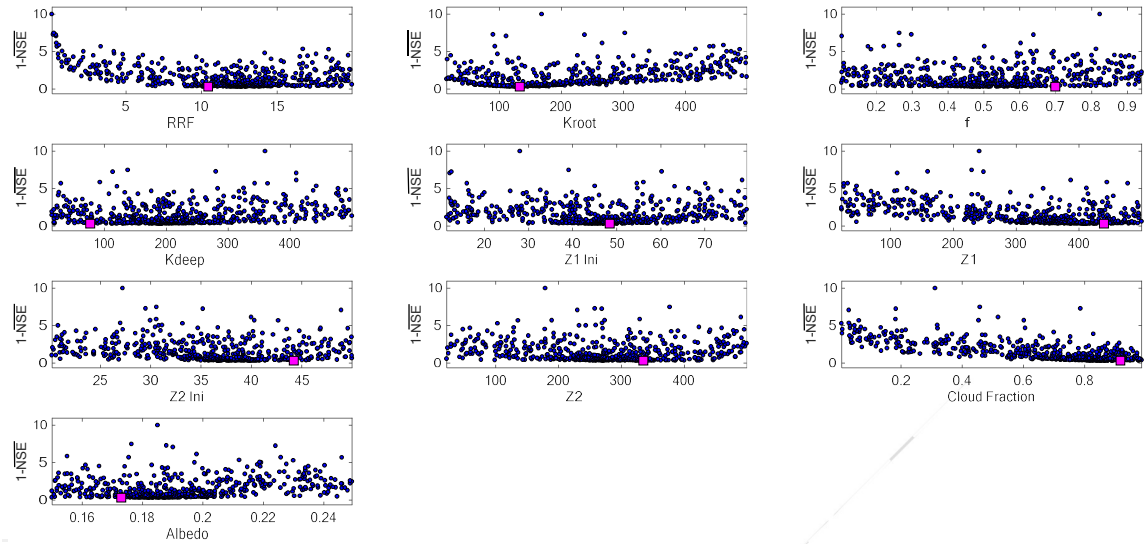

Figure 6. Dotty plots objective function (1-$\overline{NSE}$). Calibration of cluster 5.

To evaluate the sensitivity of the model parameters, the Regional Sensitivity Analysis (RSA; Homberger and Spear, 1981) was used. In this method, sensitivity is defined as the effect of the parameters on overall model performance (Wagener *et al.*, 2001a). The results show that all parameters are sensitive in the model because different parameter values affect model results (see Figure 7).

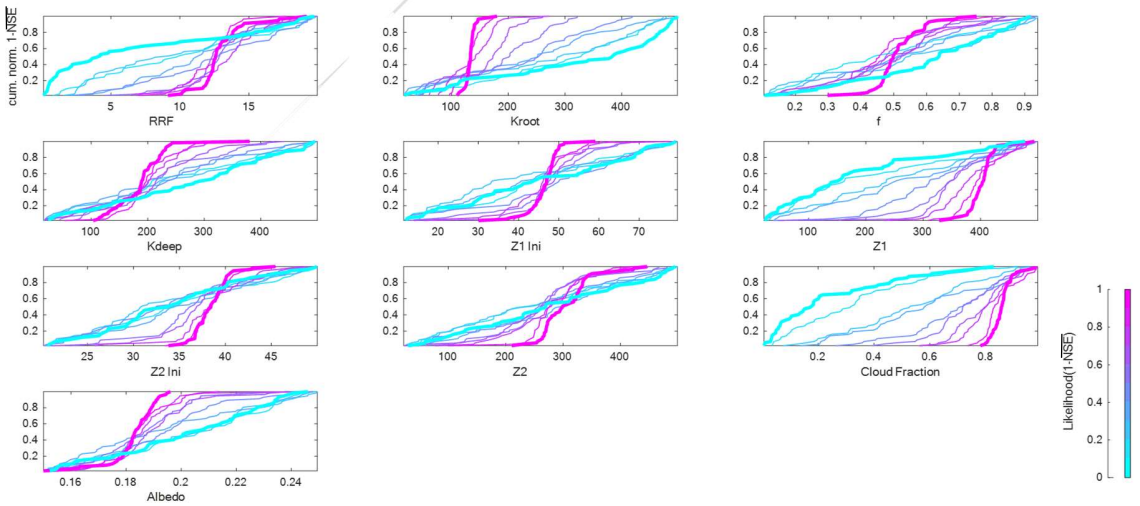

Figure 7. Regional sensitivity plot (1-$\overline{NSE}$)

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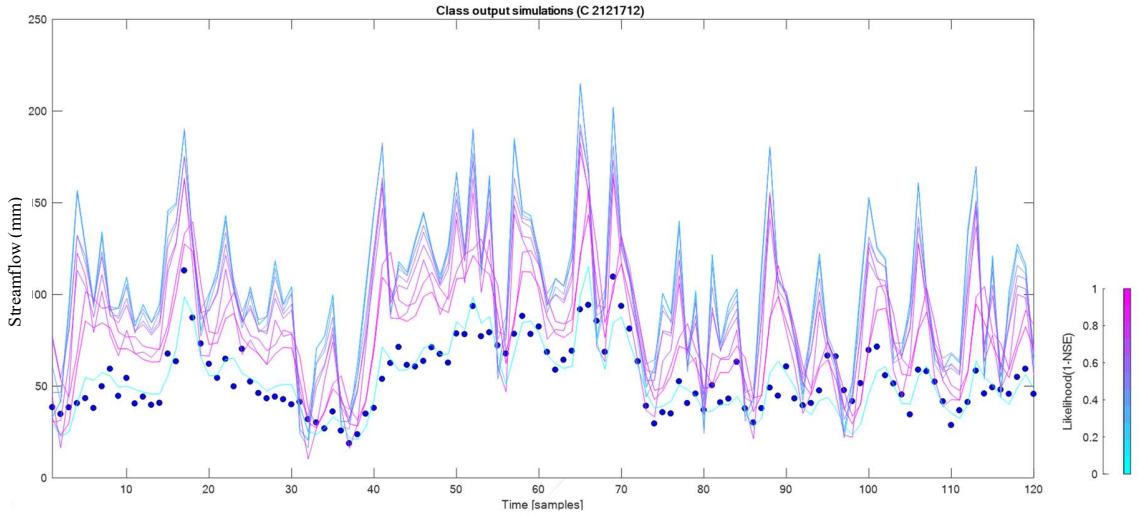
As an indication of the spread of output time-series, the class plot was used. This plot displays 10 sample simulation time series outputs, classified considering the objective function (Wagener *et al.,* 2001a). The results for sub-catchments used for calibration in cluster 5 are presented in Figure 8.



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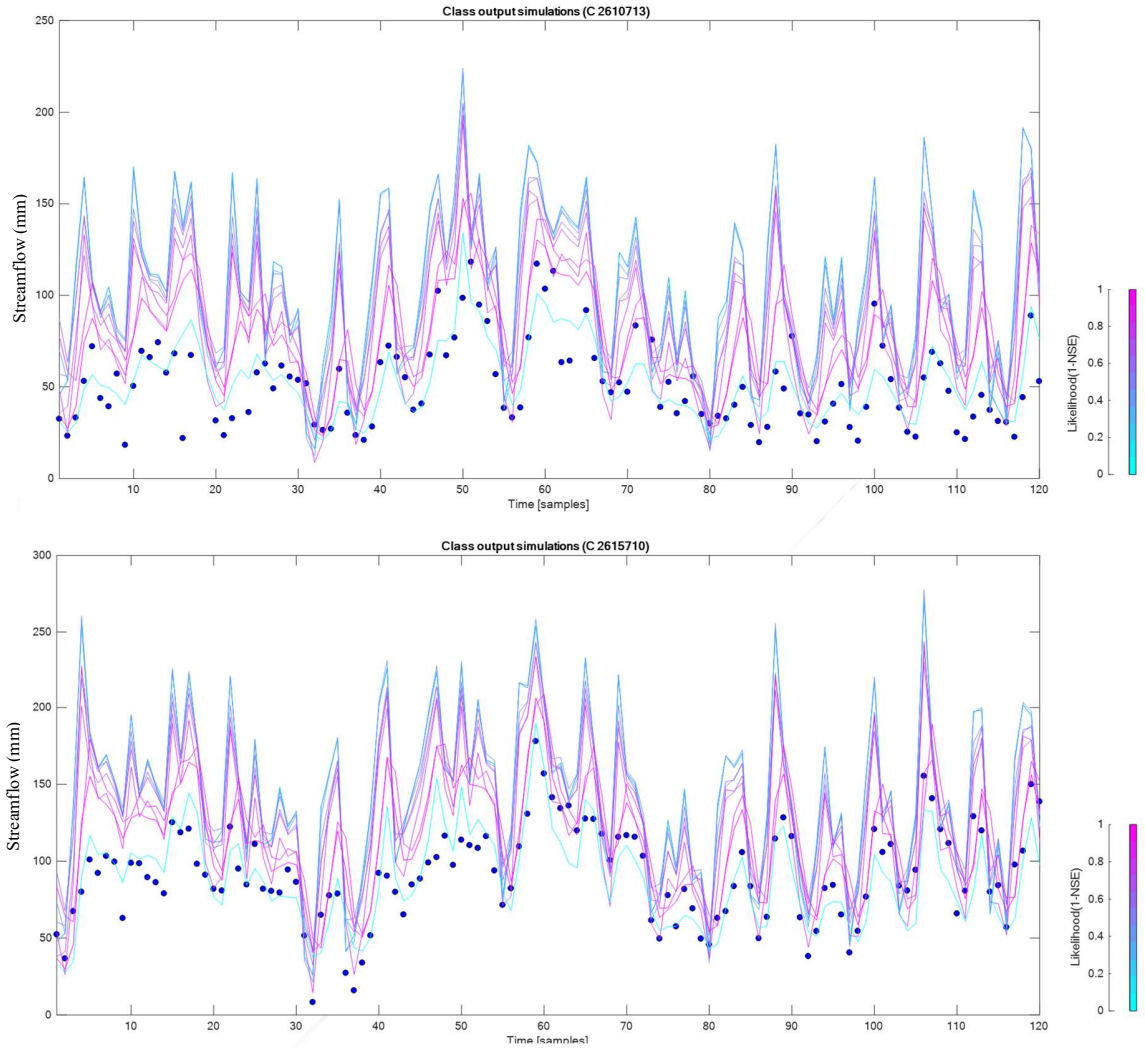

Figure 8. Class plot for sub-catchments for calibration in cluster 5

The output uncertainty was estimated using the Generalised Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992). In MCAT, the plot displays the time-series output with associated confidence intervals. As presented by Wagener *et al*. (2001a), for each point, a cumulative frequency distribution is generated using the selected objective and the confidence intervals calculated using linear interpolation. The results for sub-catchments used for calibration in cluster 5 are presented in Figure 9.

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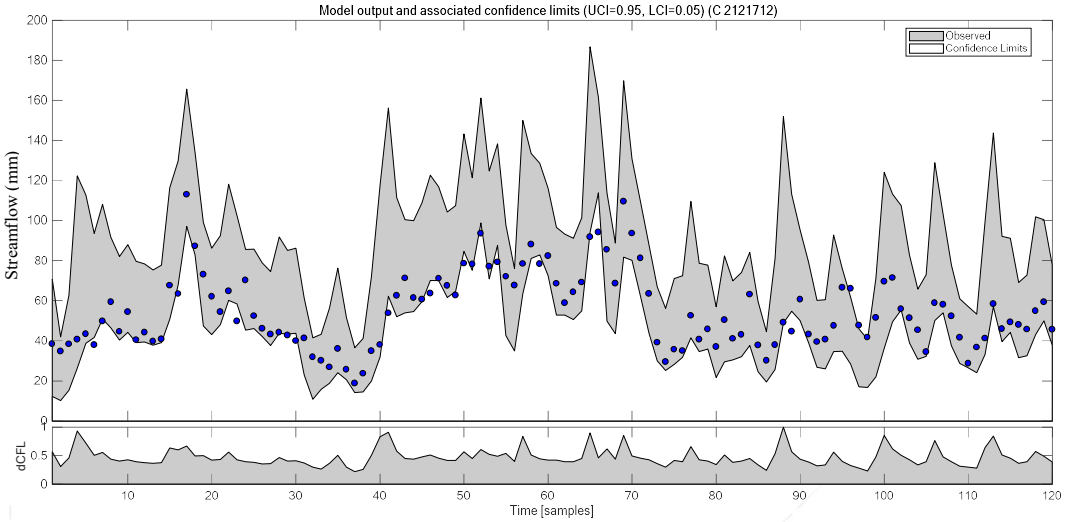

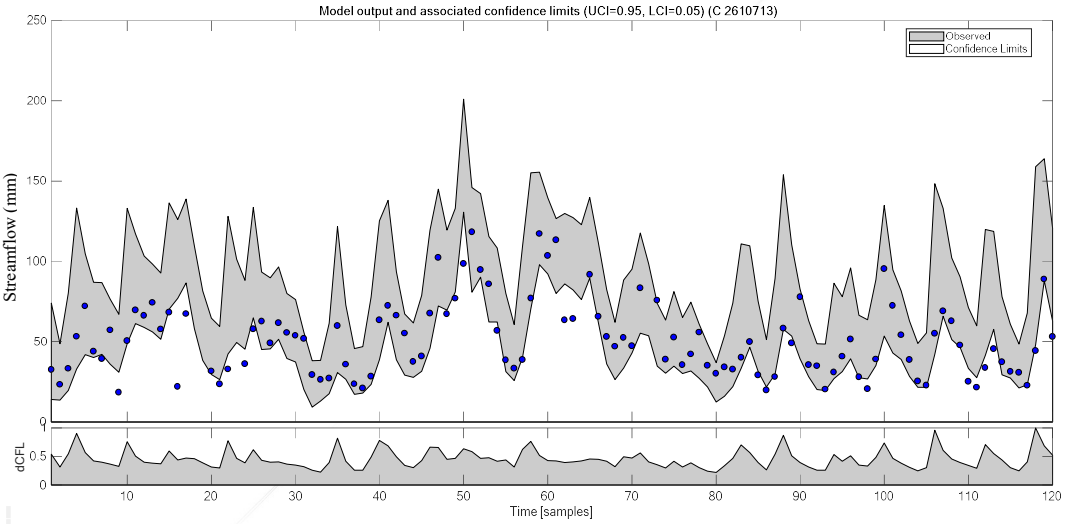

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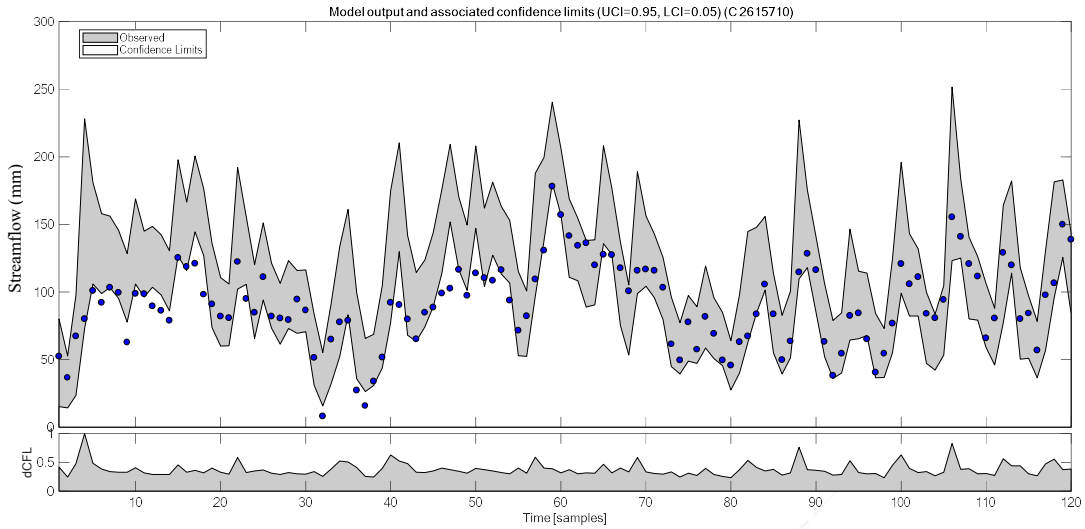

Figure 9. GLUE output uncertainty limits for sub-catchments for calibration in cluster 5

Finally, MCAT offers multi-objective plots. These are scatter plots of each objective versus every other objective function, A large scatter indicates that the objectives are unrelated, whereas a clear pattern indicates that the objective functions attempt to fit the model to the same part of the observed data (Wagener *et al.*, 2001a). The objective function names are shown in the diagonal. The plots above the diagonal shows the correlation coefficient between the objective functions. As an example, Figure 10 shows the multi-objective plot for sub-catchments 2121712, 2610713 and 2615710 with 1-NSE, APBias and RMSE objective functions.

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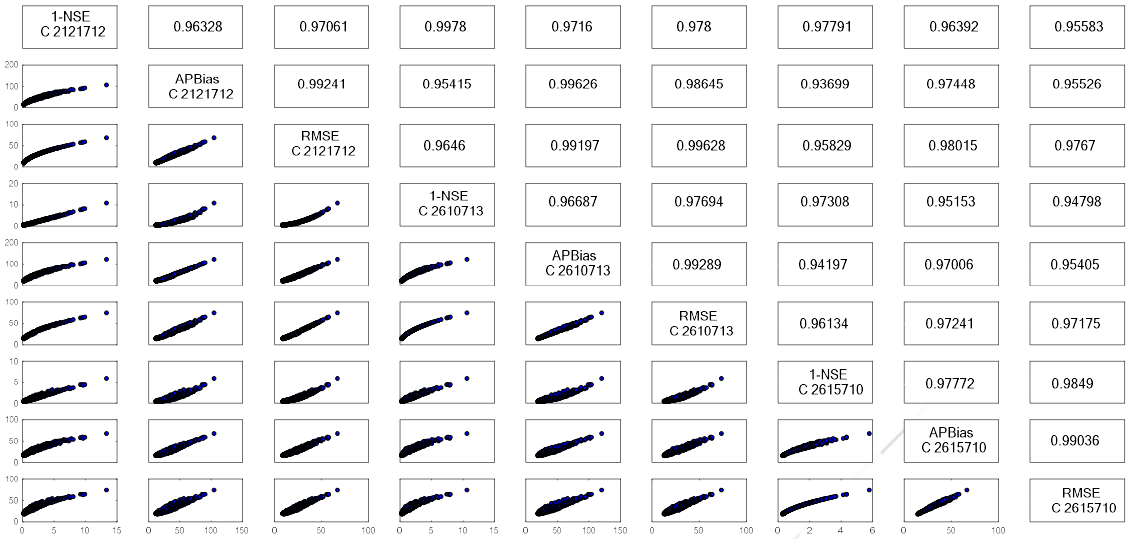

Figure 10. Multi-Objective plot

6. *Validation on data from period of times not used*

Based on the criteria proposed by Klemes (1986), a validation with split-sample was performed. The validation period was from 2005 to 2014. Table 10 presents the calculated objective functions on data for the period of time not used in calibration.

Table 10. Calculated objective functions in validation on data from period of times not used for calibration

Group	$\overline{NSE}$	$\overline{RMSE}$	$RBias_{max}$
1	0.80	550.6	-4.2%
2	0.47	347.5	-21.9%
3	0.64	562.7	5.4%
4	0.63	406.8	14.6%
5	0.51	97.8	-4.1%
6	0.43	297.4	16.1%
7	0.65	518.4	-19.1%
8	0.76	116.5	-2.8%
9	0.68	310.4	-6.9%

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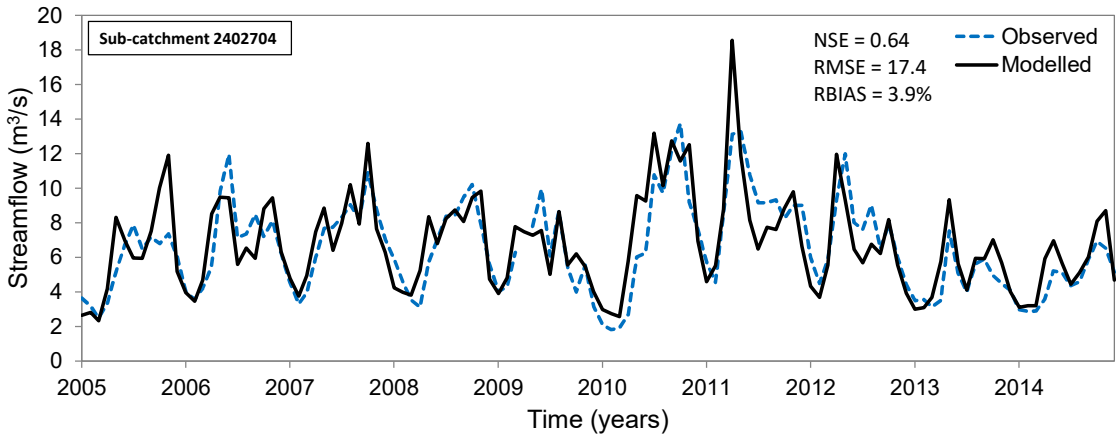
Group	$\overline{NSE}$	$\overline{RMSE}$	$RBias_{max}$
10	0.63	322.5	12.7%
11	0.75	321.0	-7.1%
12	0.83	171.6	5.9%
13	0.63	327.2	-4.4%
14	0.78	231.0	5.1%
15	0.57	506.3	-14.4%

Considering the values of the different objective functions, the results are acceptable for the validation procedure. As an example, Figure 11 presents the comparison in the validation period for the sub-catchments 2402704, 2602721 and 2602725 in cluster 10, between observed streamflow and modelled streamflow.



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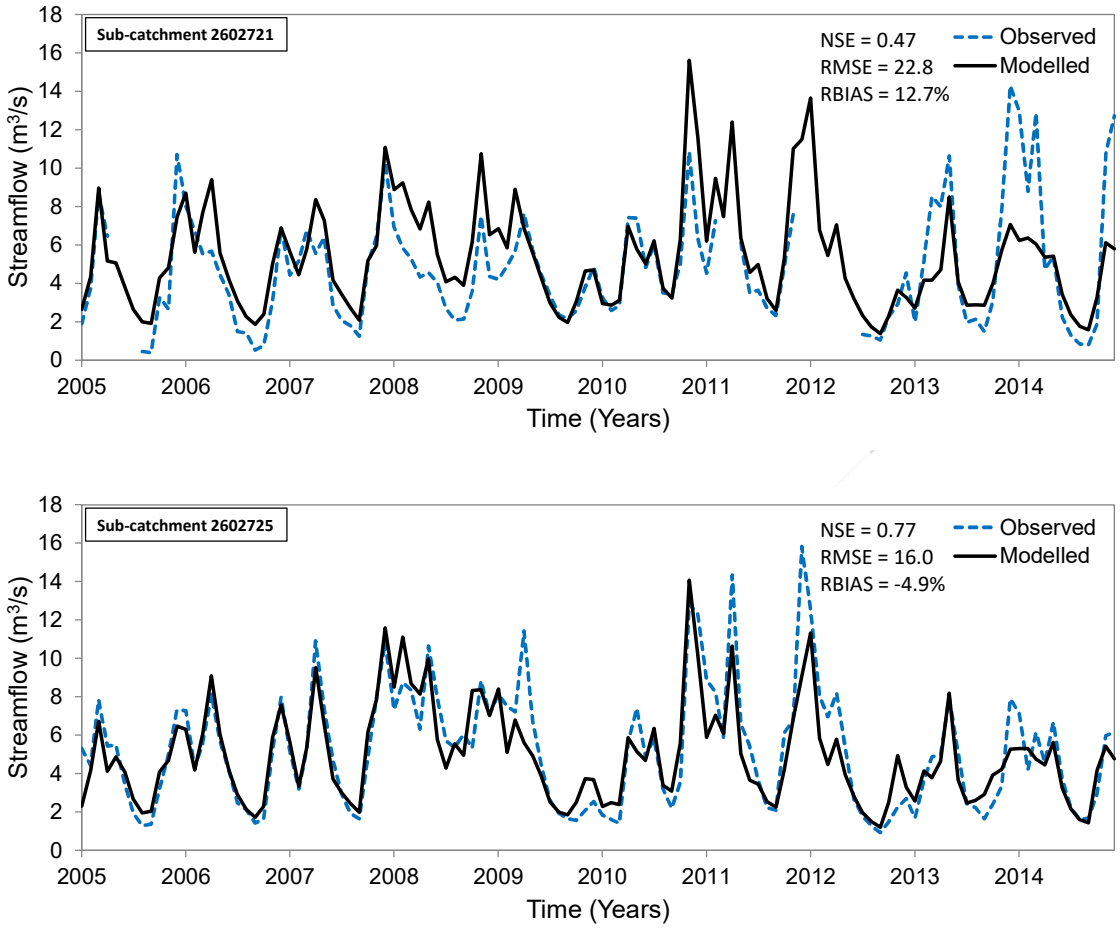

Figure 11. Validation results for sub-catchments in cluster 10

7. *Transfer calibrated parameters to sub-catchments in the defined clusters*

In this step, the parameters values presented in Table 8 were assigned to each sub-catchment of the model according to the cluster that it was in. At the end of this procedure, all sub-catchments in the model have the parameters obtained in the procedure and the model is ready for a final spatial validation based on data that are available in the model units that were not used in the calibration.

8. *Validate on data that is available in sub-catchments not used in the calibration*

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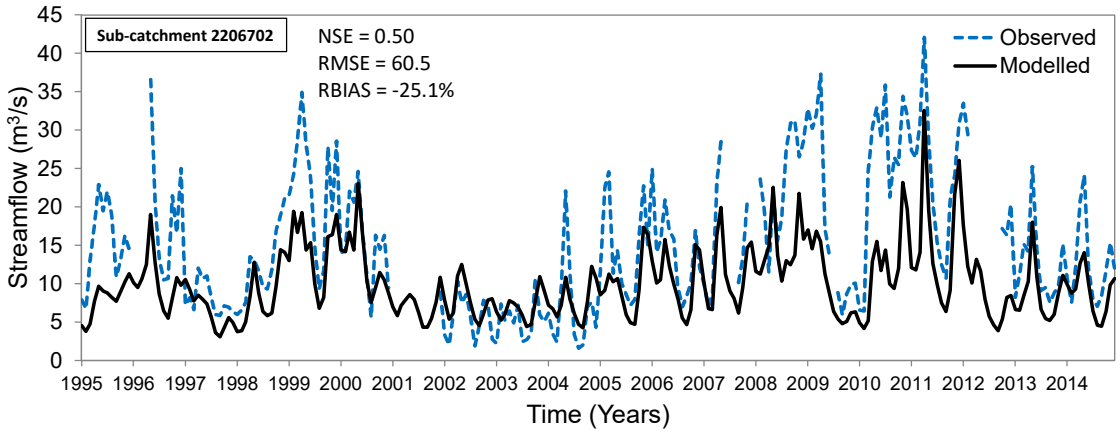
Finally, a validation on data that are available in sub-catchments not used in the calibration was performed. In the case of the WEAP Magdalena-Cauca model, only 2 clusters have information that allows this procedure (clusters 4 and 5). The calculated objective functions in this validation are presented in Table 11.

Table 11. Calculated objective functions in validation on sub-catchments not used in the calibration

Cluster	$\overline{NSE}$	$\overline{RMSE}$	$RBias_{max}$
4	0.45	470.2	-9.4%
5	0.48	371.2	-25.1%

The results obtained are acceptable and shows that the methodology is suitable for the calibration of the model. As an example, Figure 16 presents the validation for the sub-catchments 2206702, 2306708 and 2613711 in cluster 5. It is important to notice that for the validation the complete period of time was analysed from years 1995 to 2014.



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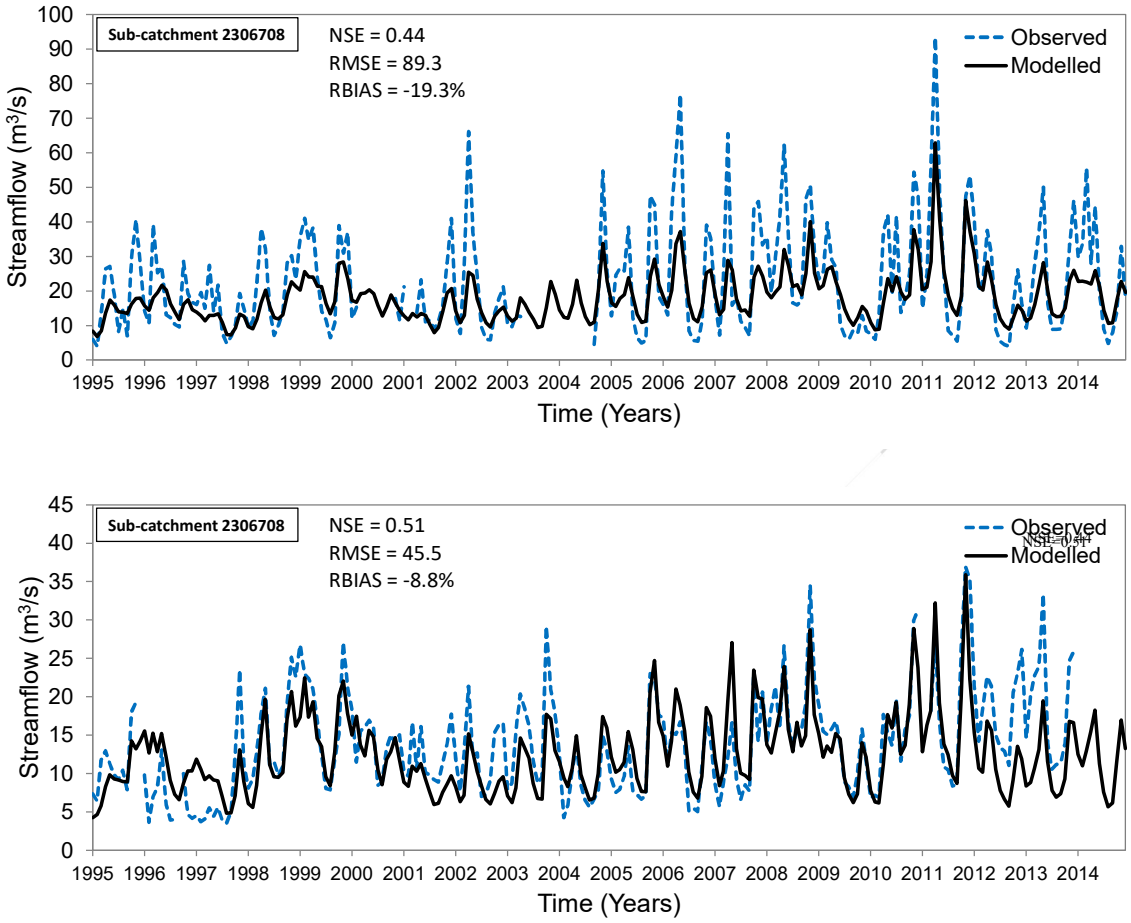

Figure 12. Validation results for group 5 on data in sub-catchments not used in calibration

4. Conclusions

In this paper a proposed methodological framework for the calibration of a large river basin hydrological model is presented. The methodology consists in 8 steps: Calculate morphometric parameters, hierarchical clustering, select a subset of sub-catchments for calibration, objective calibration, analyse calibration results and model parameter uncertainty, validation on data from period of times not used, transfer calibrated parameters to sub-catchments in the defined groups and validate on data that is available in sub-catchments not used in the calibration.

The methodology was tested in the calibration of a WEAP Magdalena-Cauca model in Colombia with acceptable results in calibration (Nash-Sutcliffe efficiency coefficient between 0.83 and 0.45) and validation (Nash-Sutcliffe efficiency coefficient between 0.83 and 0.43 in validation). In this case, the entire model units were classified in 15 groups according to the hierarchical clustering exercise. Though the Magdalena-Cauca basin is well monitored and has the best hydrological information available in Colombia, there is a lack of information and the uncertainty of the model response is from middle to high. It is important to highlight the importance of good available data for the procedure to reduce the uncertainty in the response not only in quantity, but also in quality. Other biophysical variables, such as climate, geology and land cover, may be used to complement the morphometric parameters used in this study for the clustering analysis, that could also improve the performance of the calibration framework.

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