

Reduction of computational times using the equivalent rectangle concept in the physics-based surface – subsurface models

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Abstract

The interaction between surface and subsurface domains in a basin can be studied using a physics-based model; however, the calibration and validation processes require a high computational effort due to their complex geometry. The authors propose an alternative to reduce the computational times during the calibration model by simplifying the geometry of the watershed that applies the equivalent rectangle concept. A quasi-3D equivalent rectangle is used to define the specific soil parameters of the Lerma river basin through sensitivity analysis that will later be applied in the calibration. The simplified model can highly accurately identify the parameter range for the initial values of the calibration process as well as if the reduction in running times is significant. Thus, the rectangle equivalent concept offers an alternative to speed-up the calibration of a 3-D fully-coupled surface sub-surface model.

Keywords: Equivalent rectangle; calibration; parameterization; surface-subsurface model; hydrological modeling.

Reducción de tiempos computacionales usando el concepto de rectángulo equivalente en los modelos físicos superficiales – subsuperficiales

Resumen

La interacción entre la superficie y subsuperficie de una cuenca se puede estudiar utilizando modelos físicos, pero debido a su compleja geometría los procesos de calibración y validación requieren altos tiempos computacionales. Para ello, se propone una alternativa que permita reducir los tiempos de calibración del modelo, mediante la simplificación de la geometría de la cuenca y empleando el concepto del rectángulo equivalente. El rectángulo equivalente es usado para definir los parámetros del suelo de la cuenca del río Lerma, a través de un análisis de sensibilidad, que posteriormente son empleados dentro de la calibración. El modelo simplificado identifica con una gran precisión los rangos y valores iniciales de los parámetros utilizados para los procesos de calibración y además reduce significativamente los tiempos computacionales. Por lo tanto, el concepto de rectángulo equivalente ofrece una alternativa para acelerar la calibración de modelos acoplados superficie-subsuperficie.

Palabras Clave: Rectángulo equivalente; calibración; parametrización; modelos superficial-subsuperficial; modelación hidrológica.

1. Introduction

Modeling is a basic tool in hydrology since it enables predictions and diagnoses of the basin flows and it generally takes into account the study area's environmental

characteristics. Models can be physical, analogue, or mathematical. Physical models have been very important in the past. However, the mathematical group of models is the most easily and universally applied and the one with the most rapid development regarding having a scientific basis and

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application [1]. According to the applicability and the objective of the simulation, there are different types of models that can be used (lumped, distributed, conceptual, physics-based, among others) and these accurately represent the analyzed natural system. Among these models, the fully-coupled physics-based models have arisen as useful tools to represent hydrological processes of a catchment area [2–9]. The study focused on the interaction between surface and subsurface flow in a basin using the physics-based hydrological models [10-12]. These describe water movement by solving the diffusive wave approximation of the shallow water equations in the overland flow, and are helped by Richard's equation. However, for the calibration and validation processes, these models need longer computational times due to the high temporal and spatial resolution required.

Considering the spatial accuracy needed in the model, the whole catchment area and its boundaries are discretized by several thousand grid nodes. Each node has specific values for the parameters used in the model. To reduce the number of calibration parameters, zones of homogeneous parameter values have been set; this is in order to evaluate and identify which parameters are available from field data and which ones need some fitting. An additional condition for the calibration parameter selection is that parameters must influence the model output, i.e. model predictions should be sensitive to changes in the values of the parameters: this feature is called identifiability.

In these types of models, parameters' values are estimated with a manual trial-and-error procedure since the automated calibration codes -which use mathematical optimization algorithms-, have difficulties with sparse data or require too many model runs [13]. Therefore, the modeler's experience is very important for the success and quality of the results.

Sensitivity studies are a suitable tool to quantify the influence of the initial set of parameters' values on the model outputs. Commonly, the methods use direct numerical differentiation, and the simulation repeats with a slightly different parameters value. There are two different kinds of sensitivity analysis, the first, local sensitivities, evaluates the sensitivity at one point of the parameter space and is usually applied in simple hydrological modeling cases. The second, global analysis, repeats the first method at many points of the parameter space. These processes require the previously mentioned huge computational effort; however, the physics-based models demand a high temporal and spatial resolution. Thus, a method to solve these problems is proposed using a geometrical simplifications model, where the topography and geology become simpler.

A quasi-3D equivalent rectangle model (ERM), similar to that presented in [14] is suggested as a substitute for the 3-D fully-coupled model, and it has the purpose of speeding up the parameterization and calibration processes. In this method, certain geometrical characteristics such as surface area and perimeter remain the same as in the original model, while other parameters are simplified, such as the elevation distribution of the watershed, which is represented by the hypsometric curve. The ERM may be applied to small to moderate catchments, in which the slope has an important feature in the basin and can be represented without taking

into account lateral variation in the geology.

The aim of the study is to show that the simplified proposed approximation can assess and identify the suitable parameter ranges and the respective sensitivity. It will then transfer it to a realistic model (3-D physic-based model), which will reduce computational times. The study focuses on the Lerma basin, which is located in the southeast of the Arba watershed in Spain.

2. Materials and methods

The first step before performing the calibration is to define the parameters that will be used in this process. This activity is referred to in the literature as parameterization [1], which involves a sensitivity analysis. Since calibration is typically manual is important to define relatively small parameter ranges that help to reduce the demanding computational times. Also, for the sensitivity study, it is adequate to identify the starting parameters' values (initial guess) as these help to reduce the number of iterations that are required.

Sensitivity is an important analytical tool for parameterization as it evaluates and quantifies the influence of the parameters in the model outputs. If the outputs are sensitive to the change of parameter values, the parameter is set as identifiable, which is a significant characteristic for parameterization. For most models, including the physics-based one, the sensitivities are calculated through numerical differentiation, which define the model output at a location (x) and a time (t), given a vector of parameters values \mathbf{p} with a total of parameter values (n_{par}), defined as $f = f(x, t, \mathbf{p})$. In this case, $f(x, t, \mathbf{p})$ can be a simulated hydraulic head of the subsurface domain or a simulated discharge in the surface domain. To determine sensitivities, only the model outputs at a location and time where previous data is recorded or observations have been previously made are considered. A numerical approximation of the sensitivity $\partial f / \partial p_i$ using a forward-difference scheme can be computed as:

$$\frac{\partial f(x,t,\mathbf{p})}{\partial p_i} \approx \frac{f(x,t,\mathbf{p}+e_i\Delta p_i)-f(x,t,\mathbf{p})}{\Delta p_i} \quad (1)$$

Where e_i is the standard basis vector at position i , and Δp_i is the change (increase) that is applied to each of the analyzed parameters respective to a defined variable (henceforth perturbation).

If $f(x, t, \mathbf{p})$ depends linearly on \mathbf{p} , more specifically, when small perturbations generate the same effect on the model output no matter the original parameter value, $n_{par} + 1$ simulations will be needed for the computational process. One will be used for the parameter vector \mathbf{p} and the other for the n_{par} for each parameter perturbation (small increment). Moreover, if the dependence of $f(x, t, \mathbf{p})$ on \mathbf{p} is nonlinear, the local sensitivities can vary significantly since each parameter perturbation depends not only on the perturbed value, but also on the parameters' values that are unperturbed. In this case, global sensitivity evaluation is used, for which the local sensitivities (s_i) are calculated for

different values of each parameter studied $p_i (i, i = 1, 2 \dots n_{par})$. This increases the number of required simulations.

In our surface-subsurface model, nonlinearity is present in both governing equations, the diffusive wave, and the Richards equation. If within the parameterization, global sensitivities at different parameter values are similar, nonlinearity is not a problem. However, if sensitivity of one or more parameters changes drastically, there can be many inconsistencies. It should also be pointed out that a parameter in local sensitivity could be considered unimportant in terms of hydrological response, but it may be very important in global evaluation. Thus, for the present study and for the physics-based model, the global sensitivities analysis is used for each parameter.

As previously stated, global sensitivity can also be affected by the values chosen for the remaining parameters (i.e., unperturbed parameters) [15]; therefore, the global evaluation should be repeated for several different values in parameter space for the $n_{par} - 1$ remaining parameters. These will also increase the required simulations up to $(n_{par} + 1)(s_1 s_2 x s_3 x \dots x s_{n_{par}})$. For this analysis, the computational effort is high due to the large number of simulations that are required in order to calculate an absolute global sensitivity (i.e., the total of the global sensitivity measures) in a physics-based model.

In order to estimate the global sensitivity, the Composite Scaled Sensitivities (CSS) is applied. CSS evaluates the local sensitivities for a range of parameters' values; it then groups the data, classifies each of the parameter analyzed, and finally averages the values based on the results. CSS was introduced by Hill [16] and can be expressed as [17]:

$$(CSS_i)^2 = \frac{1}{n_{obs}} [P(J^T \omega J)P] \quad (2)$$

Where n_{obs} is the total number of observations considered to calculate the composited scaled sensitivities, P is a diagonal matrix ($n_{par} \times n_{par}$) of the parameter values used to calculate the sensitivity, J is the local sensitivity matrix ($n_{obs} \times n_{par}$) containing all terms of the form $\partial f / \partial p_i$, and ω is a weighting matrix ($n_{obs} \times n_{obs}$). For the purposes of comparison, in order to evaluate the applicability of the simplified model proposed, CSS are computed for both the simplified model and the real catchment.

In conclusion, the parameterization process in the physics-based surface-subsurface model includes a global sensitivity analysis. This helps to identify the parameters that are important in model fitting and at what ranges of values these parameters are sensitive. This would help to define the correct parameter values for the calibration.

After the relevant parameters are defined, calibration is performed. The purpose of the calibration is to establish that the model can reproduce field measurements and estimate parameter values based on measured quantities. Calibration can be performed manually or automatically. While manual calibration is deemed to be subjective due to the arbitrary decision of the modeler about the performance of the model, automatic calibration may imply significant computation times that are not affordable in very complex applications.

The choice of the calibration method depends on the modeler and is conditioned by the model running time.

In order to test whether the calibrated model performs well, in the sense that the deviations between the measured and simulated values are within an acceptable range, an χ^2 -test of the objective function normalized by the covariance matrix of the error, C_{yy} , is often calculated. In particular, the optimization function $\frac{\chi^2}{DoF} = 1$ is used, where DoF is the model's degree of freedom, which is defined as the difference between the number of observations and the number of calibration parameters [11].

2.1. A quasi-3D equivalent rectangle model (ERM)

In order to reduce the computational times in the parameterization, the geometrical characteristics of the catchment were simplified by using the equivalent rectangle. What this method does is convert the watershed 3-D fully coupled model into a quasi-3-D equivalent rectangle. The model total surface area A and the perimeter P_e are preserved; these variables are useful to be able to determine the width (w) and length (l) of the ERM base plane. The solution for w and l are the following systems:

$$wl = A \quad (3)$$

$$2(l + w) = P_e \quad (4)$$

The previous equations follow the equivalent rectangle concept, which was introduced by Roche [18]. They study the influence of the geometrical characteristics of a basin on its hydrological response. However, the topographic structure is simplified into a single hillslope, which keeps the hypsometric curve of the natural basin [14]. The hypsometric curve is an empirical cumulative distribution function, $F_n(z)$, that is discretized by a digital elevation model (DEM). Since the resolution (cell size) of the DEM is known, the elevation value is associated with frequency $\frac{\Delta A}{A}$, where ΔA is the area of one DEM cell, and A is the total area of the watershed that is plotted against the elevation values z_i . The cumulative frequency $\left(\frac{\Delta A}{A}\right)$ is plotted along the abscissa and the elevation along the ordinate. This can be expressed as:

$$F_n(z) = P(x \leq z) \approx \frac{1}{u} \sum_{i=1}^u I(x \leq z) \quad (5)$$

Where u , is the DEM's number of cells and I is an indicator of a random variable, which is set to 1 when the property $x \leq z$ is accomplished. Otherwise the value is zero.

Since the rectangle is uniform in the y -direction, w is set to be uniform and a quasi-3D model is assumed. For the subsurface domain, given the DEM, the ERM can be reproduced by representing the hypsometric curve of the aquifer top and bottom surface. Thus, it assumes that vertical geometry is simple where the catchment boundaries of the surface coincide with the boundaries of the subsurface. In order to test the ERM in the parameterization process of the physics-based surface-subsurface model we used the Lerma catchment.

3. Case study: Lerma basin

The Lerma basin has an area of approximately 7.5 km² and is located south-east of the Arba catchment, which is within the Ebro basin [2,9]. The catchment is a semi-arid area that was formerly fallows land that was transformed into an irrigation agriculture catchment in 2006. It has two lithological units that are characterized by a quaternary deposit, and the overlying tertiary bedrock is made of lutites and marlstones [9]. The upper unit represents a phreatic aquifer, hereafter called “glacis”, that is seasonally fed by precipitation and irrigation (agriculture is a strong activity at the basin). The glacis has permeable characteristics, it is unconsolidated, and has clastic deposits that generally are present in arid or semi-arid climates. The tertiary unit represents an aquitard, hereafter called “buro”. This formation is relatively sensitive to weathering and fracturing processes, and there is possible filtration of water from upper layers [9]. Despite being an aquitard, the model includes the top part of this formation for the simulation.

A digital elevation model (DEM) of 25 m cell-sized was used. Hydrological information (daily rainfall, air temperature, wind velocity, relative humidity and solar radiation) was obtained from a climatological station located five kilometers from the Lerma basin. A soil characterization campaign was performed in 10 different points of the Lerma basin, in order to obtain soil properties. The samples collected (depth of one meter) were classified by different textures (clayey, clayey-loam and sandy-clayey-loam) and bulk densities. Porosities (\emptyset) were calculated from soil densities at saturated and dry conditions; specific storage (S_s) and residual water saturation ($S_{w,r}$) were defined from literature. To define hydraulic conductivities (k_s), information from a pumping test performed within the Arba catchment was used. Values obtained were between 1 and 7.7 m/d, which are larger than the ones found in the literature (0.005 and 1.0 m/d) for the same lithologic unit. To determine the van-Genuchten parameters (used in the subsurface domain, together with Richards equation), α and n , we faced some difficulties as in the literature review there are only typical values for these parameters [19,20]: α varies between 0.05 and 6.0 m⁻¹, while n is between 1.01 and 2. As previously described, the soil properties reflect a huge uncertainty in the parameter values. For this reason the hydraulic conductivity and the van-Genuchten parameters are taken into account for the parameterization process.

Another parameter that commonly has a significant influence on hydrological models is the overland flow friction coefficient. Previous investigations [21] suggest that the overland flow friction coefficient may have a very high sensitivity on the calibration of flow-coupled models. Therefore, Manning’s roughness coefficient, n_m , which is very often used to express overland flow friction, was also subject to investigation during the parameterization of the Lerma basin model.

Boundary conditions for the ERM are set to no flow except for the outlet that is defined as critical depth. This is similar to the conceptual model of the Lerma Basin presented in [2,3]. These assumptions were incorporated into the ERM in order for the results to be comparable. Subsurface

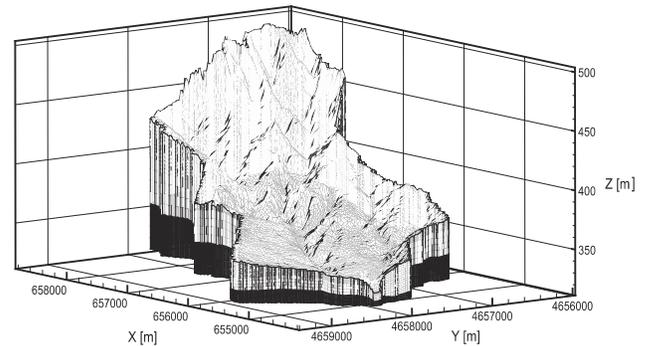
parameters were assumed to be isotropic in the whole domain. For the initial conditions of the model, the dynamic water balance approach presented by [9] was used. Following this approach, the ERM was repeatedly forced with one-year meteorological input data (rainfall and evapotranspiration) until a steady-state was reached.

4. Results

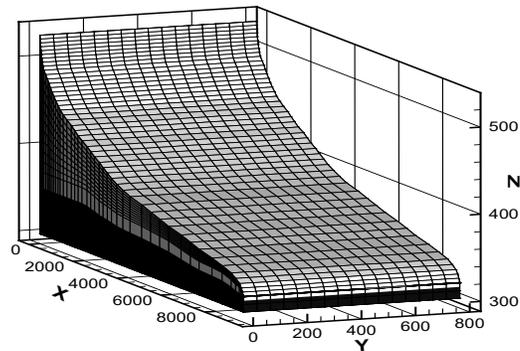
As previously mentioned, a simplification of the Lerma basin 3-D fully-coupled was performed in order to reduce the computational times in the calibration process of a physics-based surface-subsurface model. The main idea behind reducing these times was to achieve an adequate parameterization (correct choice of the calibration parameters), where a quasi-3D model based on the concept of equivalent rectangle was used to study the sensitivity of certain parameter ranges. In the simplification, the elevation distribution of the watershed is represented by the hypsometric curve.

In the ERM, glacis and buro units have uniform parameter values (area-weighted average value). This results in a simplified two-layer scheme in the subsurface structure; the first is a phreatic aquifer overlying an aquitard. Both the 3-D fully coupled model (hereafter called the complex model) and the Lerma basin ERM are shown Fig 1.

The parameters chosen for the parameterization process are hydraulic conductivity (k_s), the van Genuchten parameters,



a) Lerma basin 3D-model: gray: glacis (aquifer) and black: tertiary materials (aquitard)



b) ERM: gray: glacis (aquifer) and black: tertiary materials (aquitard)
Figure 1. Lerma basin model and the simplified model, Equivalent Rectangle (ERM)

Source: Author’s own design

Table 1.

Parameter range for the sensitivity studies of saturated hydraulic conductivity, k_s , inverse of the air entry pressure, α , pore distribution factor, n , and Manning's roughness coefficient (n-manning) for the Lerma basin.

Parameter	Min. Value	Max. Value	$d p_i$
K_s [m/d]	0.04	8.64	0.01
α [m^{-1}]	0.01	6.0	0.005
n [-]	1.0	3.0	0.05
n - Manning [$s/m^{1/3}$]	0.03	0.05	0.001

Source: Author's own design

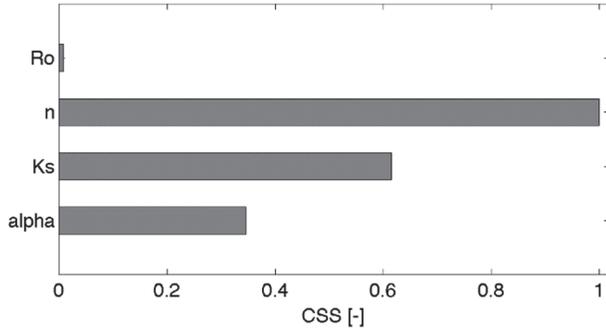


Figure 2. Composite - Scale Sensitivities (CSS) calculated using the Equivalent Rectangle Model (ERM).

Source: Author's own design

inverse air entry pressure (α), and pore distribution factor (n). The Manning's roughness coefficient (Ro) was also being investigated. Table 1 presents the range of the parameter values and the perturbation (Δp_i) used for each parameter (p_i) in the sensitivity analysis. When this analysis was performed, only physical values of the soils and predominant land-use within Lerma basin [9] were tested.

The first step in the parameterization process is to define the parameters that have a relevant effect on the hydrological response of the watershed. Thus, we undertook a sensitivity assess and then a ranking parameter (i.e. k_s , α , n and Ro) was calculated using the ERM. Larger CSS values indicate parameters that are more meaningful. CSS' Fig 2. presents the CSS normalized ranking, and it can be observed that the CSS value for Manning's roughness coefficient is very low compared to k_s , α , and n ; this is also detailed in Perez et al. [19]. Hence, the parameterization exercise presented in this paper focused on the remaining three parameters (k_s , α , and n). It is important to mention that the values of Ro used ranged from 0.03 to 0.05 as these values correspond to values are typically presented in the literature in terms of the cropping patterns associated with the Lerma Basin.

In order to speed up the calibration, it is important to narrow down the dimension of the significant parameter space and set the range for which the parameters are sensitive. In order to do this, we used multiple simulations with different parameter value combinations for k_s , α , and n . We calculated CSS values for each range of parameters, we assumed the weighting factor (ω) to be the inverse of the measurement error matrix (C_{yy}^{-1}), and we set a relative error of 10% for the discharge measurements. The results provided

a ranking for each parameter that shows the variation of the sensitivity in the parameter space (see Fig 3). This helps to reduce the parameter range for calibration and consequently the computational times. For the three rankings, it is possible to observe values for which the sensibility on the model output is higher.

To demonstrate the applicability of the ERM, the sensitivity study (CSS) was also performed using the 3-D fully coupled model of the Lerma basin with more than 200,000 elements. For a comparable analysis between these two models, the homogeneous glaciais was also assumed in the complex model. The CSS was calculated as having equivalent conditions to those used in the ERM, i.e. having equivalent combinations of parameter values, precipitation, evapotranspiration, and irrigation data. The results of the CSS values for the ERM and the 3-D fully-coupled model are shown in Fig 4.

The calculated CSS values for both models are very similar and they show the applicability of the simplification on parameter studies. According to the figure, values of CSS for the inverse of the air-entry pressure, α , are higher (around 1). They decrease around 3 and 5 and increase again for higher values of α . CSS for n show higher values around $n = 1.2$. CSS values decrease for higher values of n . For the case of k_s , CSS values slightly decrease when of k_s values increase.

To further investigate the applicability of the ERM, the model is used in the Lerma basin calibration process. [2] proposed a calibration of the Lerma basin, but as it is highlighted by [3], the approach presented is slow. In this study, the ERM is used to speed-up the calibration process.

To calibrate the model, instead of using the complex model the ERM was used. Also, values of the calibration parameters (i.e. k_s , α , and n) were systematically changed by using an automatic approach performed using the software PEST [22] within the pre-defined ranges. This was undertaken until a reasonably good performance of the model, compared to the measured data, was found. To improve the agreement between simulated and measured data, the set of calibrated parameters obtained using the ERM was introduced to the complex model. Five more iterations were then needed to achieve the model's best performance.

While with the original approach (using the complex model) more than 100 manual iterations that took 50,000 minutes were needed to achieve the best performance, the approach using the ERM that included more than 1000 automatic iterations and five iterations with the complex model only took less than 7000 minutes. This reduction in the time required to calibrate the model was more than 700%.

In Fig 5, the evolution of the performance of the model expressed as the ratio X^2/DoF is presented. As is shown, the optimal value of the ratio (best performance of the model) was reached after 1000 automatic iterations using the ERM model and five more iterations using the complex model.

Calibrated values obtained for the glaciais formation were $k_s = 0.95 m/d$, $\alpha = 0.8 1/m$, and $n = 1.54 [-]$; and for the buro formation $k_s = 0.01 m/d$, $\alpha = 1.0 1/m$, and $n = 1.35 [-]$, are very close to the average calibrated values reported by [2,3] for the glaciais and the buro.

5. Conclusions

The reduction in running times with the simplification of the watershed geometry is significant: while a single run with the 3-D fully-coupled model of the Lerma basin takes between 420 and 600 minutes, for the ERM it only takes between 3 and 8 minutes. This means, that for a sensitivity study of a physics-based superficial-subsuperficial model for a one year simulation of the Lerma basin (around 1000 runs) using a single 1.3 GHz Intel Core i5 computer, it would take around 300 days to obtain representative results. With the ERM, it would take less than four days using a computer with the same specifications. The situation appears to be worse when more layers are used, as well as when feedbacks between soil moisture and evapotranspiration are used as simulations for more than 37 hours for a single run and they have been reported for the same basin [3].

Simplification of the geometry of the basin using the rectangle equivalent concept appears to be a good approximation to speed up the calibration of 3-D fully-coupled, physics-based models.

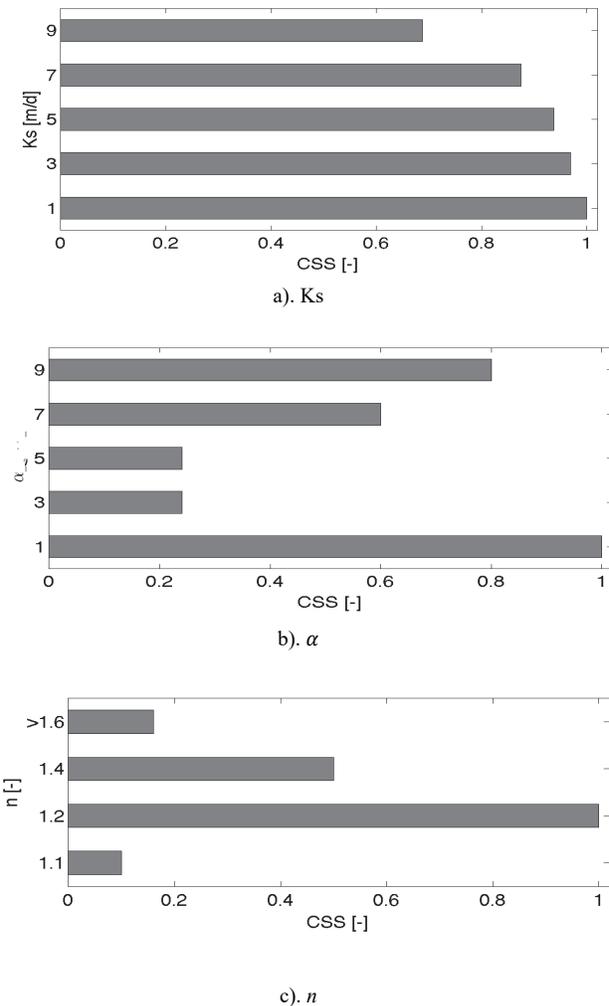


Figure 3. Sensitivity analysis using the ERM.
Source: Author's own design

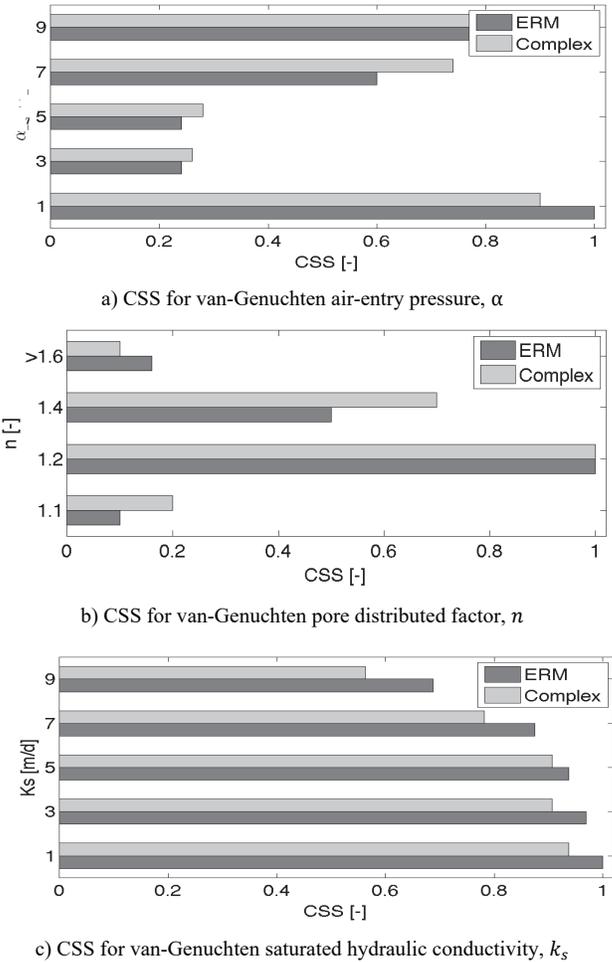


Figure 4. CSS calculated for the Lerma basin's complex and simplified models (ERM).
Source: Author's own design

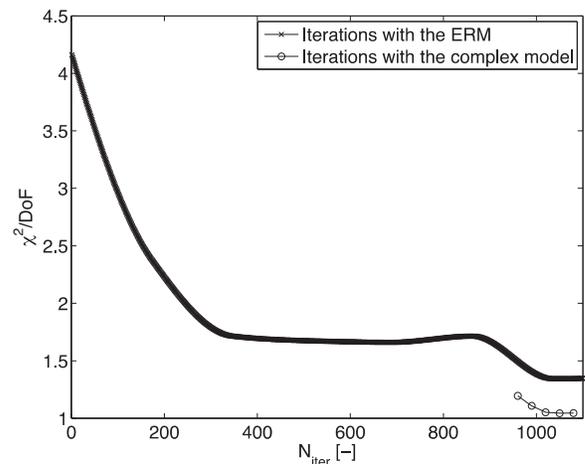


Figure 5. Calibration process using a combination of the ERM and the complex model.
Source: Author's own design

By speeding up the process, the ERM may also help to reduce subjectivity during the calibration, promote the use of

more appropriate automatic algorithms, and improve the performance of physics-based, fully-coupled hydrologic models.

Results suggest that the ERM may be applied for small to moderate catchments where the slope denotes an important feature in the basin and it can be represented without taking into account lateral variation in the geology.

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