INTRODUCTION

Physically based models are constructed according to mass, momentum and energy conservation principles [1]. The development of computer capacity made them practically applicable in the 1980s. Despite the improvement of their physical realism, physically based models suffer from extreme data request, scale-related problems (some parameters are not directly measurable) and over-parameterization. Furthermore, hydrological modeling is a difficult task because of its multiple sources of uncertainties. Apart from the uncertainty due to randomness in the natural processes that cannot be reduced, several uncertainties remain: data uncertainty, model structural uncertainty and model identifiability uncertainty. The first one corresponds to errors introduced in measurements and observations of the fields or in data pre-processing. The second one comes from the imperfect model description of real world processes. And the last one mainly results from the two others. In fact, it reveals the model inability to converge to a single optimum parameter set because of interaction between parameters resulting in multiple local optima [2]. Therefore, calibration of parameters, usually of a few key parameters, is a necessary step in the model development.

Data assimilation methods for parameter estimation can be exploited to improve parameter identification as well as the outlet flow prediction [3]. This paper focuses on variational data assimilation and more precisely the adjoint method. First studies on the adjoint approach for variational assimilation meteorological observations were realized by Penenko and Obraztsov [4] with synthetic data and were carried on by Le Dimet and Talagrand [3]. These methods are being used at the European Center for Medium Range Weather Forecasting since 1997, at the French Meteorological Service (Météo-France) since 2000, and at the National Center for Environmental Prediction (USA). They also appeared in operational oceanographic prediction. Data assimilation is now being applied with increasing frequency to hydrological problems and begins to influence the way hydrologists think about both data collection and modeling [5, 6]. Local gradient-based search techniques are widely used for parameter estimation of ground water modeling [7].

The first objective of this study is to make the best use of the available data and to capture the dominant response of the catchment, by reducing uncertainties linked to the hydrological system characterization during flash flood generation [8]. The second objective is to improve the understanding of land surface processes and mechanisms of modeling. “Understanding model behavior and performance increases the transparency of the modeling procedure and helps in the assessment of the reliability of modeling results” [9].

To achieve these objectives, an estimation of parameters, involved in the calibration of the distributed MARINE (Modélisation de l’Anticipation du Ruissellement et des Inondations pour les événements) model, is performed. The estimation procedure is based on the adjoint state theory that is an optimal control problem determining the optimal control variables. The approach employed in this paper is to use prior knowledge of the spatial variation of parameter values and to apply scalar multipliers to the maps of spatially variable parameters in order to minimize a cost function. The advantage is to reduce the dimensionality of the estimation problem. The goal is to determine scalar multipliers of the most sensitive parameters that better simulate the behavior of the watershed and effectively control the rate of infiltration and runoff over the watershed for floods of different intensities.

The paper is composed of four sections. The first one presents the adjoint state theory and introduces automatic differentiation tools. The second section describes the flash flood MARINE model and the estimation framework. Section 3 briefly lists characteristics of the catchment. Finally, an example applying the methodology to the MARINE model for the Gardon d’Anduze catchment is presented.

ADJOINT STATE THEORY

Data assimilation is part of inverse problems based on mathematical methods. In hydrology, difficulties result from non-linearities, which make the model very dependant on initial conditions. Data assimilation is the process by which observations are combined together with numerical models to produce a description of the catchment state and a prediction of the outlet flow as accurate as possible. A variational data assimilation technique called the adjoint state method is used in the MARINE model. This method comes from the optimal control theory [10].
Hydrological model can be described by a system of non-linear differential equations where the state variable $X$ describes the field, for instance the water elevation at grid points:

$$
\begin{align*}
\frac{dX}{dt} &= F(X, \Theta) \\
X(0) &= V
\end{align*}
$$

(1)

$X$ depends on time and is of large dimension. $F$ is the non-linear operator governing the evolution of the water elevation. $V$ is the initial condition and $\Theta$ is a variable which represents all the input parameters of the model. The basic principle is to consider $\Theta$ and $V$ as control variables and optimize them in order to minimize the misfit between the observations $X_{obs}$ (distributed in time and space) and solutions of the model. The cost function is a norm measuring this misfit:

$$
J(\Theta, V) = 1/2 \int_0^T \| HX(\Theta, V) - X_{obs} \|_{obs}^2 \, dt
$$

(2)

The operator $H$ is defined in such a way that $HX$ belongs to the space of observations. The problem is then formulated as determining $(\Theta, V)$ that minimize $J$. If $J$ is differentiable, a necessary condition for $(\Theta_{opt}, V_{opt})$ to be a solution of the optimization problem is given by the Euler-Lagrange equation (3).

$$
\nabla J(\Theta_{opt}, V_{opt}) = 0
$$

(3)

Optimization algorithms are used to find the optimum of the cost function. For the gradient calculation, the Gâteaux derivative formalism, a generalization of the concept of directional derivative, is employed. An auxiliary variable, the so-called adjoint variable $P$ is defined. It can be showed that if $P$ is the solution of the adjoint model:

$$
\begin{align*}
\frac{dP}{dt} + \left[ \frac{\partial F}{\partial X} \right]^T P &= H^T (HX - X_{obs}) \\
P(0) &= 0
\end{align*}
$$

(4)

Then the gradient of $J$ is given by:

$$
\nabla J = (\nabla_{\Theta} J, \nabla_{V} J) = \left[ \frac{\partial F}{\partial \Theta} \right]^T P, - P(0)
$$

(5)

where $\left[ \frac{\partial F}{\partial \Theta} \right]^T$ is the transposed Jacobian of the model with respect to the state variables. Therefore, all the components of the gradient can be calculated thanks to the adjoint variable obtained with a backward integration of the adjoint model. The adjoint state method allows an efficient calculation of the cost function gradient with respect to all control variables, with a calculation cost that does not depend on the number of variables.

**Automatic Differentiation (AD)**

The major difficulty of this method is to develop the adjoint model. And once developed, it must be validated because minor error in computing the gradient can significantly degrade the efficiency of the minimization. This difficult task can be facilitated by powerful AD tools, which are intended at automatically developing the adjoint of a given code. AD tools, based on program transformation, parse and analyze the original program (the direct code) and generate a new source program (the adjoint code). Such tools are very powerful and allow the best representation of the functional to be derived. For a more complete description of AD, the reader is referred to [11] or the community website at www.autodiff.org.

**Optimization**

An optimization algorithm is then used to estimate the optimum initial condition and input parameters. A numerical descent-type method consists in the following sequence:
\[
\begin{bmatrix}
\Theta_n \\
V_n
\end{bmatrix}
= \begin{bmatrix}
\Theta_{n+1} \\
V_{n+1}
\end{bmatrix} + \rho_n D_n
\]  

(6)

where \( \rho_n \) and \( D_n \) are the step and direction of descent respectively. This direction can be calculated with conjugate gradient or Newton type methods.

THE MARINE MODEL AND ESTIMATION FRAMEWORK

The MARINE Model

The MARINE model is a flash flood forecast model developed for real-time exploitation of small watersheds [12]. In order to better represent heterogeneities of the rainfall as well as various behaviors of the land surface, the model is spatially distributed, which also helps to understand the surface processes. MARINE can integrate remote sensing data with spatial resolution adapted to hydrological scales. The model requires a minimum number of data to run: the Digital Elevation Model from satellite SPOT which contains the catchment topography and its location; the rainfall data which come from meteorological radar (Météo France), the land cover and vegetation map (SPOT, LANDSAT) and the rivers description. The MARINE model is basically controlled by parameters listed in Table 1. The infiltration parameters and the Manning roughness coefficient come from classes of geological units: soil types (see Fig. 1) and vegetation types respectively. For each class, some parameters are either directly assessed from field data or subject to calibration. The resulting parameters are distributed according to a priori values derived from published tables and generate reference maps. The water trajectories on the land surface are deduced from the watershed slopes (DEM).

Inside this physically based model, the infiltration capacity is evaluated by the Green and Ampt equation. The infiltration rate is equal to the rainfall intensity as long as the rainfall intensity doesn’t exceed the potential infiltration rate. When the rainfall rate goes beyond the infiltration rate, the soil is saturated and ponding occurs. The infiltration rate \( I \) into vertically homogeneous columns at the local scale is expressed as:

\[
I(t) = \begin{cases} 
P / K (1 + \psi / (\theta_s - \theta_i)) & , \quad t \leq t_p \\
F(t) / \theta_s & , \quad t > t_p 
\end{cases}
\]  

(7)

where \( P \) is rainfall rate, \( t_p \) is time to ponding, \( K \) is the saturated hydraulic conductivity, \( \theta_i \) and \( \theta_s \) are the initial and saturated soil water content respectively. \( \psi \) is the soil wetting front suction and \( F \) is the cumulative infiltration.

The surface runoff calculation is divided in two parts: the land surface flow and the flow in the drainage network, both based on the hypothesis of the kinematic wave. For the overland flow representation of small watersheds during flash flood, the kinematic wave approximation is supposed to be valid [13]. The overland flow equation results from a combination between the mass conservation equation and the Manning’s friction equation:

\[
\frac{\partial h}{\partial t} + \frac{5}{3} S h^{2/3} \frac{\partial h}{\partial x} = P - I
\]  

(8)

where, \( h(x,t) \) represent the water depth at point \( x \) and time \( t \), \( S = S(x) \) and \( n = n(x) \) are the principal land surface slope and the Manning roughness coefficient at the point \( x \) respectively. The forcing function on the right hand side, difference between the rainfall and soil infiltration rate, represents the rainfall excess available for the surface runoff.

Fig. 1. Soil classes and soil depth of the catchment
Table 1. Input parameters for the MARINE model

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Name</th>
<th>Spatial distribution</th>
<th>Data sources</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial soil moisture (%)</td>
<td>$\theta_i$</td>
<td>yes</td>
<td>SIM</td>
</tr>
<tr>
<td>Soil depth (m)</td>
<td>$Z_x$</td>
<td>yes</td>
<td>BRGM</td>
</tr>
<tr>
<td>Infiltration parameters:</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- hydraulic conductivity (mm/h)</td>
<td>$K_x$</td>
<td>yes</td>
<td>Soil classes</td>
</tr>
<tr>
<td>- porosity (%)</td>
<td>$\theta_s$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>- wetting front suction (mm)</td>
<td>$\psi_x$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Manning roughness coefficient (m$^{1/3}$ s)</td>
<td>$n_x$</td>
<td>yes</td>
<td>Vegetation classes</td>
</tr>
<tr>
<td>Drainage network</td>
<td>Manning roughness coefficient (m$^{1/3}$ s)</td>
<td>$n_d$</td>
<td>no</td>
</tr>
</tbody>
</table>

The Estimation Framework

A cost function, measuring the misfit between simulations and observations, is defined and implemented into the MARINE model. A wide range of cost functions is available, their choice remains a subjective decision depending on the specific application the modeler wants to focus on [14]. Herein, the cost function is defined as follows:

$$J(\Theta) = \frac{1}{m} \sum_{i=1}^{m} \left( Q_{obs}^i - Q_{sim}^i(\Theta) \right)^2 \left/ \sum_{i=1}^{m} \left( Q_{obs}^i - \overline{Q}_{obs} \right)^2 \right.$$  

(9)

where $\Theta$ is the calibration parameters, $m$ is the total number of observations, $Q_{obs}^i$ and $Q_{sim}^i$ are the observed and simulated discharge at time step $i$ respectively. Viewing the calibration parameter as control variables, the estimation process consists in minimizing $J$ with an optimization algorithm. Optimization problem using quasi-Newton method (BFGS) presents two main advantages. Firstly, the method is robust and efficient for distributed models. Secondly, it is adapted to the minimization of non-smooth cost functions [15]. Therefore, a quasi-Newton algorithm with inequality constrains from the MODULOPT library was chosen in this study [16]. The adjoint code of MARINE, necessary for cost function gradient calculation, is given by TAPENADE [17], a differentiation automatic tool distributed by INRIA and developed since 1999. The adjoint code is validated by the “dot test product” and by comparing the results with divided differences.

CASE STUDY

The previously described methodology is applied on the Gardon d’Anduze catchment, located in southern France. This Mediterranean catchment, of 545 km² drainage area, is often affected by flash floods. It is part of a hydrological rainfall runoff model intercomparison project leaded by the French central hydrometeorological service for flood forecasting (SCHAPI).

Drainage System:

The hydrological network is dense. The Gardon d’Anduze catchment is divided in two subbasins: the Gardon de Mialet and the Gardon de Saint-Jean. Their confluence, two kilometers before the outlet, constitutes the entire basin. The Gardon is steep-sided river and its longitudinal slope is higher than 1.5%.

Topography:

The upper part of the catchment corresponds to the high Cévenol basin characterized by a mountainous region with peaks, narrow valleys, steep hillslopes and several torrential flow streams. Near the catchment outlet located at Anduze, hillslopes are less important (2%) and the riverbed becomes larger within an alluvial plain. The highest areas are found in the Cévennes, where the elevation rises up to 1200m a.s.l. near the mount Aigoual and the outlet is located at approximately 130m a.s.l. A DEM data file of the study site with a grid scale of 50m is available from the French national geographic institute (IGN – BD TOPO®). The mean slope of the whole basin is approximately 20%.

Soils:

The major part of the catchment area (64%) is developed on metamorphic terrain. The substrate is made of shale and crystalline rocks overlain by silty clay loams (83%) and sandy loam top soil [18]. Soil types data were available from the BDSol-LR. These data have been used to generate the initial distribution of the infiltration parameters.

Vegetation and land use:

Vegetation is dense and typical of Mediterranean forests, composed mainly of chestnut trees, pasture, Holm Oaks, conifers, waste land and garrigue. A land-use classification from SPOT satellite is used to generate the initial distribution of the roughness coefficient on the hillslopes. Land use map is used to derive distributed surface roughness.
Climate:
The Gardon region is characterized by the highest rainfall intensities recorded in France. The conjunction of high intensity rainfall, shallow soils and steep slopes produce very devastating floods in autumn even if summer storms can also present a non-negligible flooding risk. Radar rainfall measurements are available with a spatial resolution of 1 km².

Observations:
The available observations are flood hydrographs at the outlet of the catchment.

RESULTS

Parameter Estimation

Researchers observed that it is not possible to locate a meaningful global optimum in the feasible parameter space for different model structures [19]. They suggested that in the presence of errors in data or model structure, the notion of a global model optimum is not appropriate [20]. Finally, they replaced the idea of uniqueness of a parameter set by an approach based on interval or regional identifiability of possible parameter sets [21]. In order to avoid the “non-uniqueness problem” and reduce the dimensionality of the identification problem, studies on sensitivity analysis based on GLUE (Generalised Likelihood Uncertainty Estimation) method were implemented [2]. Results of those studies showed that the most sensitive parameters are hydraulic conductivity ($K$), soil depth ($Z$) and the high flow drainage network roughness coefficient ($n_d$). The first two parameters are used to calculate the infiltration rate. The last one ($n_d$) controls the runoff routing through the watershed to the basin outlet. However, it is necessary to reduce the high dimensional space due to the spatial distribution of parameters. Hence, the parameter estimation process is achieved by using two scalar multipliers $C_K$ and $C_Z$ to adjust the magnitude of hydraulic conductivity and soil depth maps while preserving their spatial distribution. Consequently the study focuses on determining scalar multipliers $C_K$, $C_Z$ and the constant roughness coefficient of the high flow channel $n_d$.

The following example presents results obtained for the flood which occurred in September 2000 and corresponds to a medium event, with a peak discharge of 1184 m³/s. The estimation framework is detailed on Table 2. Ranges of scalar multipliers are adjusted with the intent of preserving physically realistic parameter values. Evolutions of parameter values during the cost function convergence are illustrated in Fig. 2. Results show a good convergence of parameters for a reasonable number of iterations. Moreover, final value parameters are physically acceptable and are well inferior to their respectively upper-bounds. The mean value of $K$ on the catchment, initially 0.65 cm/h, becomes 4.43 cm/h after adjustment. Values of $K$ can be found in tables from [22]. They vary from 0.06 cm/h to 23.56 cm/h. Values of Manning’s roughness coefficient for various kinds of channels can be deduced from tables in [23]. For instance, the estimated value ($n_d = 0.096$) corresponds, for natural streams, to very weedy reaches or deep pools or for steep slopes, $n = 0.090$ for orchard. Inside the Marine model, infiltration excess dominates the flood generation (excess saturation overland flow). Consequently, it is necessary to increase the soil depth in presence of quartz, like in the upper part of Gardon d’Anduze catchment, to force infiltration capacity in those regions.

![Fig. 2. Convergence of parameters and cost function (logarithmic scale) during the minimization](image-url)
Furthermore, the evolution of parameters values during the cost function convergence gives information about the importance of each parameter with respect to the modeling process. After a fast increase at the beginning of the minimization, $C_Z$ reaches a value close to the estimated one. This important variation has an influence on the cost function convergence, which presents a similar evolution at the beginning. This shows that $C_Z$ is a sensitive parameter. The parameter $n_d$ decreases regularly and reaches its estimated value after ten iterations. After a little artifact, it finally settles to its estimated value. This parameter is also sensitive because it quickly reaches its final value. $C_k$ appears to be the less sensitive parameter since its convergence is more progressive than the other parameters. Finally, the parameters convergence gives information about their respective sensitivity. The more sensitive is the model to a parameter, the greater is the identifiability of this parameter and, the faster the cost function converges to its minimum value.

Fig. 3 shows that the increase of distributed hydraulic conductivity and soil depth values increases the infiltration rate, and reduces the water volume available for runoff. The adjustment of the high flow channel roughness coefficient contributes to a better estimation of the time of the peak discharge. Results show the efficiency and performance of the method to estimate model parameters and the simulated hydrograph is very close to the observations ($J_{\text{Nash}} = 0.049$).

**Sensitivity Analysis**

The implementation of this sensitivity analysis after the estimation process aims at determining if the parameters estimated previously are well identified. Therefore, the sensitivity analysis achieved is a very simple one, based on Monte Carlo (MC) simulation [24], which consists in sampling the parameter space with a uniform distribution. This method assumes no prior knowledge on parameters values, other than their lower and upper bounds. The tested parameters, their respective range and the sampling strategy are summarized in Table 3. Fig. 4 shows scatter plots of Nash criterion results for each parameter in MC simulation. The optimum value of each parameter is determined by the maximum value of the Nash criterion ($Nash = 1 - J$). The hydraulic conductivity is the less sensitive parameter. There is no significant optimum value for $C_k$, however, it has to be higher than roughly 3. $C_Z$ goes through a maximum value equal to 4 and lightly tends to decrease. Optimum $n_d$ values are clearly defined, and are centered on 0.1. On the whole, results of MC simulation bring same conclusions as the estimation process about relative sensitivities of parameters. Otherwise, the previously estimated set of parameter corresponds to the best MC simulation values (see Table 4). In conclusion, the estimated set of parameters with the adjoint method is consistent and gives good performance.

Table 3. Parameter ranges used in MC simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Minimum value</th>
<th>Maximum value</th>
<th>Sampling Strategy</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_k$</td>
<td>0</td>
<td>10</td>
<td>Uniform</td>
</tr>
<tr>
<td>$C_Z$</td>
<td>0</td>
<td>10</td>
<td>Uniform</td>
</tr>
<tr>
<td>$n_d$</td>
<td>0</td>
<td>20</td>
<td>Uniform</td>
</tr>
</tbody>
</table>

Fig. 4. Parameter population resulting from the MC simulation. The Nash criterion is plotted against each parameter.
Table 4. Comparison of best Monte Carlo simulation and parameter estimation process values

<table>
<thead>
<tr>
<th>Estimation process</th>
<th>C_K</th>
<th>C_Z</th>
<th>n_d</th>
<th>Nash</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monte Carlo 1</td>
<td>6.76</td>
<td>4.39</td>
<td>0.096</td>
<td>0.951</td>
</tr>
<tr>
<td>Monte Carlo 2</td>
<td>9.11</td>
<td>4.16</td>
<td>0.101</td>
<td>0.946</td>
</tr>
<tr>
<td>Monte Carlo 3</td>
<td>5.73</td>
<td>4.04</td>
<td>0.124</td>
<td>0.939</td>
</tr>
</tbody>
</table>

SIMULATION OF OTHER FLOODS

In order to validate estimated parameters, simulations of two other floods were run and compared with observations. The first, flood of September 1994, is a medium one. The second, flood of September 2002, is an exceptional one. The couple (\(C_K, C_Z\)) is the one previously estimated. However, the use Manning friction flow equation for the runoff modeling, implies that the high flow channel roughness coefficient may depend on the water level. The \(n_d\) value is less important for more intense event of similar description because of less resistance. Hence, it was necessary to estimate \(n_d\) for those new floods. Parameters and intensity of floods are summarized in Table 5. The time and intensity of the peak discharge are well estimated for the listed set of parameters, as shown in Fig. 5. Hence, the estimation process is an efficient method to determine a set of parameter capable to simulate floods of different intensities. However, to better represent the rising flow and recession phase, the model can be improved by representing subsurface hydrodynamics.

Table 5. Parameters of simulation

<table>
<thead>
<tr>
<th>Year</th>
<th>(Q_{\text{max}}) (m³/s)</th>
<th>C_K</th>
<th>C_Z</th>
<th>n_d</th>
</tr>
</thead>
<tbody>
<tr>
<td>1994</td>
<td>775</td>
<td>6.76</td>
<td>4.39</td>
<td>0.161</td>
</tr>
<tr>
<td>2002</td>
<td>3634</td>
<td></td>
<td></td>
<td>0.085</td>
</tr>
</tbody>
</table>

Fig. 5. Hydrographs simulated (solid line) compared to observations (circle symbols).

CONCLUSION

Processes involved in the transformation of rainfall forcing to hydrological response are complex. Hence, their analysis and control are very challenging. In distributed models, some parameters are not directly measurable and others need to be calibrated. Adjoint techniques are nowadays exploited in hydrology. Their practical implementation is facilitated by the advent of very efficient automatic differentiation tools. The major advantage of this method is the fact that the computational cost is independent of the number of control variables. However, due to equifinality, the performance of a sensitivity analysis is profitable before assimilation of observations for parameter and state estimation.

The first objective of this study was to determine an optimum set of parameters. Herein, local gradient-based method appears to be efficient and robust even if the highly non-linear hydrological phenomena and so the possible numerous local optima of the objective function, motivate some authors to use global search method algorithms (like the population-evolution-based search strategies [25] and genetic algorithms [26]). This study demonstrates that the methodology employed may be used to parameterize and calibrate fully distributed physically based models, and is capable of making reliable forecasts. Furthermore, the evolution of parameter values during the cost function convergence gives information about the importance of each parameter with respect to the modeling process. Consequently, this methodology contributes to: (i) improve flash flood generation understanding, (ii) validate the physical hypothesis used in the model or (iii) improve its physical representation. In the MARINE model, the rising flood and recession phase should be improved by the introduction of subsurface flows.

From an operational point of view, the objective is to implement this methodology into real-time forecasting models in order to estimate event-based input factors, such as initial soil moisture and rainfall forcing. By the way, assimilation of
observations during the rising flood phase should allow anticipation, early identification and quantification of an imminent flood and should contribute to the construction of a hydro-meteorological prediction chain.

REFERENCES