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1 Objective Functions for Conceptual Hydrological Model
2 Calibration: Theoretical Analysis of Distance- and Weak
3 Form-Based Functions

4 V. Guinot*, B. Cappelaere, C. Delenne, D. Ruelland

5
6 HydroSciences Montpellier UMR 5569 (CNRS, IRD, UM1, UM2)

7 Université Montpellier 2

8 CC MSE

9 34095 Montpellier Cedex 5

10 France

11
12 * : Corresponding author

13 e-mail : guinot@msem.univ-montp2.fr

14 Tel : +33 (0)4 67 14 90 56

15 Fax : +33 (0)4 67 14 47 74

16 **Abstract**

17 Calibrating conceptual hydrological models is often done via the optimization of
18 objective functions serving as a measure of model performance. Most of the objective
19 functions used in the hydrological literature can be classified into distance- and weak
20 form-based objective functions. Distance- and weak form-based objective functions can
21 be seen respectively as generalizations of the square error and balance error. An analysis
22 of the objective functions shows that: (i) the calibration problem is transformed from an
23 optimization problem with distance-based objective functions into a root finding problem
24 for weak form-based functions; (ii) weak form-based objective functions are essentially
25 less prone to local extrema than distance-based functions; (iii) consequently, they allow
26 simple gradient-based methods to be used; (iv) parameter redundancy can be assessed
27 very simply by superimposing the contour lines or comparing the gradients of two
28 objective functions of similar nature in the parameter space; (v) simple guidelines can be
29 defined for the selection of the calibration variables in a conceptual hydrological model.
30 The theoretical results are illustrated by two simple test cases. Weak form-based
31 approaches offer the potential for better-posed calibration problems, through the use of a
32 number of independent criteria that matches the dimension of the identification problem.
33 In contrast with distance-based objective functions, they do not have the inconvenience of
34 solution non-uniqueness. Finally, the need for models with internal variables bearing a
35 physical meaning is acknowledged, as well as the need for an a posteriori check of the
36 validity of the warm-up period.

37 **1. Introduction**

38 Calibration is recognized as an essential step in the operation of conceptual,
39 hydrological models. It is classically translated into an optimization problem, whereby an
40 objective function expressing the goodness-of-fit of the model, must be minimized or
41 maximized depending on the definition. Although several authors have pointed out the
42 importance of seeing calibration as a multi-objective optimization exercise using
43 variables and criteria of different natures (Yapo et al., 1998; Gupta et al., 1998, Meixner
44 et al., 1999), it is still conducted as a single-objective optimization procedure in a vast
45 majority of practical applications. The same holds for model performance assessment that

46 is often performed using the same type of objective functions as those used in the
47 calibration process. Such analyses are usually performed on the basis of empirical
48 considerations, for which formal foundations are lacking. Although there is a commonly
49 shared perception of the calibration/validation exercise in the hydrological community,
50 this lack of theoretical bases often does not allow reliable guidelines to be derived.

51 The present paper focuses on two types of objective functions: so-called distance-
52 based and weak form-based (or integral) objective functions (see Section 2 for a
53 definition). The purpose is to analyse the behaviour of such functions and to determine
54 under which conditions some may be better-suited than others. The choice of the model
55 variable(s) to be used in the calibration process is also discussed. The behaviour of
56 distance-based and weak form-based objective functions is analysed theoretically and
57 illustrated by two simple case studies.

58
59 Distance-based objective functions represent the vast majority of objective functions
60 used in hydrological modelling (Kavetski et al., 2006b; Schaefli and Gupta, 2007).
61 Distances may be defined for the original (Kavetski et al., 2006a) or transformed flow
62 variables. In Hogue et al. (2000, 2006) and Kavetski et al. (2006b), a logarithmic
63 transformation error is presented. The Nash-Sutcliffe Efficiency (NSE) criterion (Nash
64 and Sutcliffe, 1970), based on a Square Error (SE) measure of distance, is definitely the
65 most widely used objective function in hydrological modelling. It is a normalized variant
66 of the Least Square Estimator (LSE), and gives equivalent information to that given by
67 the Mean Square Error (MSE), or Root Mean Square Error (RMSE). A number of
68 theoretical justifications can be provided for the NSE. For instance, the NSE optimum
69 corresponds to the Maximum Likelihood Estimator for a homoscedastic, gaussian
70 distribution of model errors (Cacuci, 2003). This justifies its use in model performance
71 evaluation and uncertainty assessment techniques such as the GLUE approach (Beven
72 and Binley, 1992; Beven, 1993; Romanowicz and Beven, 2006). The NSE can also be
73 seen as the sum of three indicators (Murphy, 1998; Weglarczyk, 1998) involving the
74 correlation coefficient between the measured and modelled variable, as well as a measure
75 of conditional and unconditional bias. Gupta et al. (2009) provided another
76 decomposition of the NSE involving the correlation, the bias and a measure of variability
77 in the measured and modelled signals. Such decomposition substantiates the proposal by
78 Taylor (2001) that model performance should be assessed using both a measure of
79 distance (such as the normalized standard deviation of the bias) and the correlation
80 between observations and model outputs.

81 The NSE is not the only possible measure of distance. In Perrin et al. (2001) the Mean
82 Absolute Error (MAE) is proposed. It can be normalized into a dimensionless index such
83 as the volumetric efficiency (Criss and Winston, 2008). In Legates and McCabe (1999),
84 the Nash-Sutcliffe efficiency criterion is generalized by replacing the square of the
85 deviations with a power to be adjusted by the modeller. The purpose is to balance the
86 larger weight given to large flow values (that are often measured with the larger
87 imprecision) by using a power smaller than 2 (Krause et al., 2005).

88 Lin and Wang (2007) use the inverse of the SE and the NSE for computing
89 respectively the efficiency of chromosomes and the objective function in a genetic, global
90 optimization algorithm. Several objective functions may also be defined for low flows or
91 peak flow events, so as to allow for multiobjective calibration (Madsen, 2000; Madsen et
92 al., 2002). Multiobjective calibration may also be carried out using variables of different
93 natures (such as response signatures, see Pokhrel et al. (2008)). A review of multi-
94 objective calibration approaches can be found in Efstradiadis and Koutsoyiannis (2010).
95 Conversely, multiple distance-based objective functions may be aggregated into a single
96 one (Madsen et al., 2002; Cappelaere et al., 2003; Schoups et al., 2005). Additional
97 information may be brought by integral criteria such as the bias (Hogue et al., 2006;
98 Schoups et al., 2005), volume error (Madsen, 2000), also called Cumulative Error (CE)

99 (Perrin et al., 2001). To overcome the deficiency of the original GLUE method in
100 reflecting modelling uncertainty, more formal derivations of likelihood functions (eg.,
101 Schoups and Vrugt, 2010) or empirical adaptations of the approach (Cappelaere et al.,
102 2003, Xiong and O'Connor, 2008) have been proposed.

103 Distance-based objective functions are well-known to introduce local minima in
104 model response surfaces (Freedman et al., 1998; Skahill and Doherty, 2006; Xiong and
105 O'Connor, 2000). In Freedman et al. (1998), distance-based objective functions such as
106 the Least Squares Estimator (LSE) and the Heteroscedastic Maximum Likelihood
107 Estimator (HMLE) are shown to introduce local extrema in the objective functions of a
108 sediment transport model, thus introducing the need for global optimization or objective
109 function exploration algorithms (see e.g. Brazil and Krajewski, 1987; Goldberg, 1989;
110 Nelder and Mead, 1965; Skahill and Doherty, 2006; Duan et al., 1992). Modelling
111 experiments where the LSE and HMLE were used to calibrate and validate different
112 models on the same data indicated that the choice of the objective function plays a
113 significant role on the final, calibrated parameter values (Gan et al., 1997).

114
115 Weak form-based objective functions are somewhat less popular, as indicated by the
116 inventory in Appendix A. The best-known weak form-based objective functions are the
117 Cumulative Error (CE) (Perrin et al., 2001), also called Volume Error (Madsen, 2000),
118 and the Balance Error (BE) (Perrin et al., 2001). The BE is nothing but a scaled version of
119 the CE. The flow variable used in the CE and BE is usually the discharge at the outlet of
120 the modelled catchment. The optimal value of the BE/CE is zero. The BE/CE may be
121 used either as a constraint (typically, $CE = 0$) in a single objective optimization process or
122 as an objective function in a multiple objective calibration exercise (see e.g. Ruelland et
123 al., 2009). That the BE/CE is only a particular case and can be generalized so as to
124 generate a wider family of weak form-based objective functions has been little
125 investigated in the literature. This is one of the aspects explored in this paper.

126 The question also arises of whether using additional variables (such as model internal
127 variables) allows the calibration problem to be better constrained. Examples of this
128 approach applied to conceptual models can be found in Seibert et al. (2002), Werth et
129 al. (2009) and Winsemius et al. (2006).

130
131 The present paper deals with objective functions for conceptual hydrological models
132 that can be described by first-order differential equations. The main objectives are to (i)
133 generalize the formulation of weak form-based objective functions, (ii) analyze the
134 respective behaviour of distance-based and weak form-based objective functions and the
135 resulting degree of difficulty in the calibration exercise, (iii) investigate whether certain
136 model variables (e.g. internal variables or output fluxes) bring more information than
137 others in the calibration of model parameters.

138
139 In Section 2, distance-based and weak form-based objective functions are defined and
140 a mathematical justification is proposed for them.

141 In Section 3, the behaviour of such objective functions when applied to conceptual
142 models is analyzed. Weak form-based objective functions are shown to be more
143 monotone and less prone to local extrema than distance-based objective functions. Simple
144 rules for detecting parameter redundancy are given and guidelines are provided for the
145 choice of calibration variables.

146 Sections 4 and 5 provide two application examples. In Section 4, a single reservoir
147 model is considered and synthetic time series are used in order to avoid any possible site-
148 dependent bias. In Section 5, a three-reservoir model is applied to a Western African
149 catchment.

150 Section 6 is devoted to a discussion and concluding remarks.

151 2. Objective Function Definition

152 2.1 Introduction

153 Consider a model in the form

$$154 \quad \frac{dU}{dt} = f(U, \varphi, t) \quad (1)$$

155 where U is the state variable, t is the independent variable (in hydrological modelling,
156 the time coordinate), φ a parameter to be calibrated, and f is a known function of U , t and
157 φ . The standard calibration approach consists in comparing the variable U or a function
158 $F(U)$ of U with an observed variable $V(t)$ over a certain domain $\Omega = [t_1, t_2]$ and adjusting
159 φ in such a way that U (or $F(U)$) is « as close as possible » to V . In what follows, the
160 function F is assumed to be a monotone function of U and φ . This assumption is verified
161 by many models such as conceptual models, where F can be, for instance, taken as the
162 discharge Q that is a function of U (see Section 4). In the general case, where F is not
163 necessarily a physical function but any scaling function, it is chosen monotone in order to
164 avoid several values of $F(U)$ for a given value of U .

165 The question then arises of how the closeness between U (or $F(U)$) and V should be
166 assessed via an objective function. If the model is perfect, the output U or $F(U)$
167 reproduces exactly the variations of the measured variable V , that is, $U = V$ or
168 $F(U, \varphi) = V$ for all t over the time interval Ω (the issue of data accuracy and measurement
169 precision is not considered in the present work). In practice, this is never the case and the
170 purpose of the calibration procedure is to bring the difference $(U - V)$ or $(F(U, \varphi) - V)$ as
171 close to zero as possible. Two types of objective functions are examined hereafter:
172 distance-based and weak form-based objective functions.

173 2.2 Distance-based objective function

174 The distance-based approach is the most widely used in hydrological modelling. In
175 this approach, the objective function is defined as one of the following two functions

$$176 \quad J = a + b \|e\|_{\Omega} = a + b \|U - V\|_{\Omega} \quad (2a)$$

$$177 \quad J = a + b \|e\|_{\Omega} = a + b \|F(U, \varphi) - V\|_{\Omega} \quad (2b)$$

178 where a and b are respectively an offset and a scaling constant, e is the modelling error,
179 defined as the difference between the modelled and observed variable, and the operator
180 $\| \cdot \|$ has the properties of a norm (Courant and Hilbert, 1953):

$$181 \quad u(t) = 0 \quad \forall t \in \Omega \Leftrightarrow \|u\|_{\Omega} = 0 \quad (3a)$$

$$182 \quad \|ku\|_{\Omega} = |k| \|u\|_{\Omega} \quad \forall k \in \mathfrak{R} \quad (3b)$$

$$183 \quad \|u + v\|_{\Omega} \leq \|u\|_{\Omega} + \|v\|_{\Omega} \quad (3c)$$

184 In other words, the objective function J provides a measure of the distance between
185 the model output U or $F(U, \varphi)$ and the measurement V . Property (3a) provides a
186 fundamental justification to the distance-based approach. If the model is perfect (that is, if
187 it allows the observed variable V to be reproduced exactly), the error e is zero over Ω and
188 the objective function J is a , which is the extreme possible value. Conversely, if J is a ,
189 the model is perfect. In practice, J is never equal to a because the model is not perfect.
190 However, J can be optimized by adjusting φ suitably, hence the need for optimization
191 procedures.

192 If the data used in the calibration process is discrete (e.g. daily, weekly or monthly
193 hydrographs), the norm is computed using a discrete sum. If the data can be considered a

194 continuous function of time, the norm is computed using an integral. In what follows,
 195 only continuous functions of time will be considered for the sake of conciseness.
 196 However, the conclusions drawn for such functions remain valid for discrete model
 197 outputs.

198
 199 Examples of distance-based objective functions are given in Appendix A. The Nash-
 200 Sutcliffe Efficiency (NSE), the Square Error (SE), the Root Mean Square Error (RMSE),
 201 the Mean Absolute Error (MAE), the Volumetric Efficiency (VE) or the Generalized
 202 Nash-Sutcliffe Efficiency (GNSE) presented in the appendix can be recast in the form (2)
 203 via a proper definition of the constants a and b . The NSE gives exactly the same
 204 information as the SE, only the offset and scaling differs. The same remark holds for the
 205 MAE and VE.

206

207 Note that:

208

209 (R1) Eq. (2a) is a particular case of Eq. (2b). Eq. (2a) provides a measure of distance
 210 between the modelled state variable U in the model and the measured one, V . It is
 211 recalled that, in most applications of hydrological models, however, the variable
 212 used in the objective function is not the state variable U itself (e.g. the water depth
 213 in one of the model reservoirs) but a function of it (e.g. the output discharge).
 214 Consequently, Eq. (2b) is the most widespread form of objective function used.

215 (R2) The function F in Eq. (2b) may also include a transformation in the variables. For
 216 instance, in some applications the logarithm, or square root of the discharge, is
 217 deemed a more appropriate variable than the discharge itself because it gives more
 218 weight to low flows.

219 (R3) The objective function may be defined for a specific range of the observed (or
 220 modelled) variables. For instance, two different values of the objective function
 221 may be computed over a given period, one for low flows and another one for high
 222 flows (see e.g. Perrin et al., 2001). In this case, a weighting function $w(V)$ is used,
 223 which is nonzero only over a subset of Ω , and the norm can be written as

$$224 \quad \|e\| = \left[\int_{\Omega} w(V) |F(U, \varphi) - V|^p dt \right]^{1/p}, \quad p > 0 \quad (4a)$$

$$225 \quad \|e\| = \left[\sum_i w(V_i) |F(U_i, \varphi) - V_i|^p \right]^{1/p}, \quad p > 0 \quad (4b)$$

226 where $w(V)$ is a weighting function, equal to 0 or 1 depending on whether V is
 227 considered to belong to the category of low [high] flows, and i is the record
 228 number. Eqs. (4a) and (4b) are respectively the continuous and discrete versions of
 229 the norm. In what follows, the continuous form (4a) will be used for the sake of
 230 notation consistency, but the reader should keep in mind that the discrete form (4b)
 231 may be used instead without loss of generality. The conclusions derived using the
 232 formulation (4a) also hold for the formulation (4b) of the objective function.

233 (R4) In Eq. (4), any positive weighting function w may be used over Ω . The simplest
 234 possible case is $w = \text{Const}$, but non constant, positive functions of V , U , $F(U)$
 235 and/or t may also be considered.

236 (R5) The distance-based objective functions presented in Appendix A are particular
 237 cases of Eq. (4), where the norm of the modelling error is defined as a power of its
 238 absolute value, called a p -norm. In the NSE and SE objective functions, $p = 2$,
 239 while $p = 1$ in the MAE and VE. In the GNSE, p may be set to any value, which

240 does not necessarily have to be an integer. However, other definitions may be
 241 proposed for the norm. For instance the maximum of the modelling error over the
 242 domain Ω also verifies the definition (3a) for a norm:

$$243 \quad \|e\| = \max_{\Omega} \left[|F(U, \varphi) - V| \right] \quad (5)$$

244 Note that the power $1/p$ in Eqs. (4a-b) is not indispensable but allows Eq. (3b) to be
 245 verified.

246 (R6) The calibration process is an optimization process.

247 **2.3 Weak form-based objective function**

248 The weak form-based approach uses the property

$$249 \quad e(t) = 0 \quad \forall t \in \Omega \quad \Leftrightarrow \quad \int_{\Omega} e v \, dt = 0 \quad \forall v(t) \quad (6)$$

250 where $v(t)$ is a function defined over Ω . In what follows, v is defined as $v = w|e|^{p-1}$ for the
 251 sake of similarity with Eq. (4). This leads to the following definition for the weak form-
 252 based objective function

$$253 \quad J_p = a + b \int_{\Omega} w |e|^{p-1} e \, dt, \quad p \geq 0 \quad (7)$$

254 where a and b are respectively an offset and scaling parameter, and w is a positive
 255 weighting function defined over Ω . The Volume Error/Cumulative Error (CE) and the
 256 Balance Error (BE) presented in Appendix A are particular cases of Eq. (7) with $p = 0$
 257 and $w(t) = 1$. In contrast with the distance-based approach, the objective function defined
 258 in Eq. (7) is not necessarily positive.

259 The following remarks may be made:

260

261 (R7) Equation (7) is a particular case of (6) obtained for the specific choice $v = w|e|^{p-1}$ of
 262 the weighting function. Other formulations may be considered for v . The formula
 263 proposed in (7) has the advantage that it bears similarity with familiar distance-
 264 based objective functions (only an absolute value operator needs to be modified).

265 (R8) The calibration procedure is transformed into a root finding problem. The most
 266 desirable value for the objective function is the offset value a .

267 **3. Sensitivity Analysis for Conceptual Models**

268 **3.1 Assumptions – preliminary remarks**

269 Consider a model obeying Eq. (1). The specific form of (1) examined hereafter is

$$270 \quad \frac{dU}{dt} = R(U, t, \varphi) - g(U, \varphi) \quad (8a)$$

$$271 \quad U(t_1) = U_1 \quad (8b)$$

272 where g is a known function of U and φ , and R is a known function of U , t and φ . In
 273 conceptual models, R represents the recharge, or inflow, and g represents the outflow.

274

275 The following assumptions are made:

276 (A1) R and g are positive over Ω :

$$277 \quad R(t, \varphi) \geq 0 \quad \forall t \in \Omega \quad (9a)$$

$$278 \quad g(t) \geq 0 \quad \forall t \in \Omega \quad (9b)$$

279 (A2) The difference $R - g$ is a decreasing function of U and a monotone function of φ .

$$280 \quad \frac{\partial}{\partial U}(R - g) \leq 0 \quad \forall U \quad (10a)$$

$$281 \quad \operatorname{sgn} \left[\frac{\partial}{\partial \varphi}(R - g) \right] = \text{Const} \quad \forall \varphi \quad (10b)$$

282 (A3) There always exists a positive, steady state solution, that is, a value of U_0 for which
283 the outflow g is equal to the inflow R :

$$284 \quad \exists U_0 > 0, \quad g(U_0, \varphi) = R(U_0, t, \varphi) \quad \forall (t, \varphi) \quad (11)$$

285 (A4) $U(t_1)$ is positive:

$$286 \quad U(t_1) \geq 0 \quad (12)$$

287
288 Assumptions (A1)–(A4) are typical of conceptual, conceptual models (see Section 4).
289 When these assumptions hold, U is positive over the domain Ω (see Section B.1 in
290 Appendix B for the proof).

291
292 The sensitivity of U with respect to φ is defined as $s = \partial U / \partial \varphi$. The governing
293 equation for s is obtained by differentiating (8) with respect to φ :

$$294 \quad \frac{ds}{dt} = \frac{\partial}{\partial \varphi}(R - g) + s \frac{\partial}{\partial U}(R - g) \quad (13a)$$

$$295 \quad s(t_1) = 0 \quad (13b)$$

296 where the initial condition $s(t_1) = 0$ is derived considering that $U(t_1) = U_1$ is known and
297 does not change with φ .

298
299 It can be shown (see Section B.2 in Appendix B for the proof) that if $\partial R / \partial \varphi - \partial g / \partial \varphi$
300 keeps the same sign for all t , s has the same sign as $\partial R / \partial \varphi - \partial g / \partial \varphi$:

$$301 \quad \left. \begin{array}{l} \frac{\partial R}{\partial \varphi} - \frac{\partial g}{\partial \varphi} \leq 0 \quad \forall t \in \Omega \\ s(t_1) = 0 \end{array} \right\} \Rightarrow s(t) \leq 0 \quad \forall t \in \Omega \quad (14a)$$

$$302 \quad \left. \begin{array}{l} \frac{\partial R}{\partial \varphi} - \frac{\partial g}{\partial \varphi} \geq 0 \quad \forall t \in \Omega \\ s(t_1) = 0 \end{array} \right\} \Rightarrow s(t) \geq 0 \quad \forall t \in \Omega \quad (14b)$$

303 **3.2 Distance-based objective function**

304 Consider a distance-based objective function using the definition (4) for the norm of
305 the modelling error:

$$306 \quad J_p = a + b \int_{\Omega} w |F(U, \varphi) - V|^p dt \quad (15)$$

307 where $U(t)$ obeys (8), F is a monotone function of U as mentioned in Section 2.1 and w is
308 a strictly positive weighting function over the domain Ω . Then the derivative of the
309 objective function with respect to φ is given by one of the following two formulae
310 depending on whether the function F involves the parameter φ .

$$311 \quad \frac{dJ_p}{d\varphi} = bp \int_{\Omega} w |F(U, \varphi) - V|^{p-2} [F(U, \varphi) - V] \frac{\partial F}{\partial U} s \, dt \quad \text{if } \frac{\partial F}{\partial \varphi} = 0 \quad (16a)$$

$$312 \quad \frac{dJ_p}{d\varphi} = bp \int_{\Omega} w |F(U, \varphi) - V|^{p-2} [F(U, \varphi) - V] \left(\frac{\partial F}{\partial U} s + \frac{\partial F}{\partial \varphi} \right) dt \quad \text{if } \frac{\partial F}{\partial \varphi} \neq 0 \quad (16b)$$

313 Since the sign of s is constant (see Section 3.1) and F is assumed to be monotone, the
 314 product $\partial F / \partial U s$ keeps the same sign over Ω . Two possibilities arise:

- 315 – F is not a function of φ . In this case, Eq. (16a) is applicable. The terms
 316 $|F(U, \varphi) - V|^{p-2}$ and $\partial F / \partial U s$ in the integral keep a constant sign over Ω , while
 317 the second term $F(U) - V$ may change sign. There is a possibility for $\partial J_p / \partial \varphi$ to
 318 cancel, which is a desirable property because the purpose of the calibration
 319 exercise is to find an optimum of the function J_p .
- 320 – F is a function of both U and φ . Then, Eq. (16b) is applicable. In the case of
 321 conceptual models (see Section 4), the sign of $\partial F / \partial U s + \partial F / \partial \varphi$ is not
 322 necessarily constant because $\partial F / \partial U s$ and $\partial F / \partial \varphi$ may have opposite signs.
 323 Then both $[F(U, \varphi) - V]$ and $\partial F / \partial U s + \partial F / \partial \varphi$ in the integral may change sign.
 324 In the general case, the two terms do not cancel for the same value of φ , thus
 325 increasing the possibilities for the appearance of local extrema.

326
 327 In both cases, using a strictly positive weighting function w minimizes the number of
 328 extrema for J_p .

329 3.3 Weak form-based objective function

330 Consider a weak form-based objective function defined from Eq. (7) :

$$331 \quad J_p = a + b \int_{\Omega} w |F(U, \varphi) - V|^{p-1} [F(U, \varphi) - V] \, dt \quad (17)$$

332 with the same assumptions on F , U and w as in Section 3.2. Then

$$333 \quad \frac{dJ_p}{d\varphi} = bp \int_{\Omega} w |F(U, \varphi) - V|^{p-1} \frac{\partial F}{\partial U} s \, dt \quad \text{if } \frac{\partial F}{\partial \varphi} \neq 0 \quad (18a)$$

$$334 \quad \frac{dJ_p}{d\varphi} = bp \int_{\Omega} w |F(U, \varphi) - V|^{p-1} \left(\frac{\partial F}{\partial U} s + \frac{\partial F}{\partial \varphi} \right) dt \quad \text{if } \frac{\partial F}{\partial \varphi} \neq 0 \quad (18b)$$

335 As in Section 3.2, two possibilities arise:

- 336 – F is not a function of the parameter to be calibrated φ . In this case, $\partial F / \partial \varphi = 0$ and
 337 Eq. (18a) is applicable. Since $\partial F / \partial U s$ keeps the same sign over Ω , the sign of
 338 $\partial J_p / \partial \varphi$ cannot change. No local extremum can appear in the objective function.
- 339 – F is a function of both U and φ . Then Eq. (18b) applies. The sign of
 340 $\partial F / \partial U s + \partial F / \partial \varphi$ is not necessarily constant, as shown in Section 4. This may
 341 lead to local extrema in J_p . Nevertheless, the derivative of J_p as defined by
 342 Eq. (18b) is less prone to sign change than that defined in Eq. (16b) because the
 343 term $w |F(U, \varphi) - V|^{p-1}$ keeps a constant sign.

344 **3.4 Choice of calibration variables**

345 In the light of the expressions derived in Subsections 3.2 and 3.3, the following
346 remarks may be made:

- 347 (R9) When calibrating a given model parameter, it is not advised to use a flow variable,
348 the calculation of which involves this parameter. For instance, in a linear
349 conceptual model, the output discharge is defined as kU , where U is the water level
350 in the reservoir and k is the discharge coefficient. Using U as a calibration variable
351 for k is advisable, while using the discharge kU to calibrate k may generate local
352 extrema in the objective function. Conversely, the discharge kU may be used to
353 calibrate the effective catchment area.
- 354 (R10) In many situations however, the only variable available for measurement is not U
355 but a function of U (for instance, the outflowing discharge). In conceptual models,
356 the internal, state variable U of the model is almost never used in
357 calibration/validation procedures, while the discharge, that is only a function of U ,
358 is used in almost all situations. Then using a weak form -based objective function
359 minimizes the probability of finding local extrema compared to a distance-based
360 objective function. Consequently, classical gradient-based methods may be used
361 with a larger probability of success to find the zero of the weak form-based
362 objective function than in finding the global optimum of a distance-based objective
363 function.
- 364 (R11) Owing to the presence of $\partial F / \partial U$ and $\partial F / \partial \varphi$ in Eqs. (16b) and (18b), using such
365 a function F in the objective function, rather than the primary model variable U ,
366 has a strong influence on the direction of the gradient of the objective function in
367 the parameter space. Using several variables of different natures (or
368 transformations of the measured flow variables), such as water levels and
369 discharges, to calibrate the models, may be more beneficial and more helpful in
370 removing indeterminacy than using several objective functions on the same flow
371 variables. This was already stated in Beven (2006) about the ill-posed character of
372 the calibration exercise.
- 373 (R12) Models with several reservoirs in series have a similar behaviour with respect to
374 the objective function. Indeed, when a reservoir discharges into another, its outflow
375 discharge $g(U, \varphi)$ is the recharge $R(U, t, \varphi)$ of this second reservoir and
376 Assumptions (A1–4) still hold. Remarks (R9) and (R10) also hold for the
377 calibration of parameters governing the internal fluxes between several reservoirs
378 in a model.

379 **3.5 Objective functions as indicators of parameter redundancy**

380 Assume that two parameters φ_1 and φ_2 in the model are redundant. In this case, for any
381 given variation in φ_1 , at least one alternative value can be found for φ_2 such that the
382 modelling result remains unchanged. In other words, in the parameter subspace $\varphi_1 \times \varphi_2$,
383 there exists a relationship in the form

$$384 \quad d[F(U)] = 0 \quad (19)$$

385 Eq. (19) becomes

$$386 \quad \frac{\partial F(U)}{\partial \varphi_1} d\varphi_1 + \frac{\partial F(U)}{\partial \varphi_2} d\varphi_2 = 0 \quad \forall t \quad (20)$$

387 Eq. (20) defines a hypersurface in the parameter space and a curve in the subspace
388 $\varphi_1 \times \varphi_2$. On the hypersurface (20) one has

$$389 \quad dJ_p = \frac{\partial J_p}{\partial F(U)} d[F(U)] = 0 \quad \forall p \quad (21)$$

390 which means that the objective function is constant along (20). Consequently, the contour
 391 lines of the distance-based objective functions (15) obtained with different values of p
 392 never intersect. The remark also holds for weak form-based objective functions (17).

393 An easy way of detecting the redundancy in two model parameters is to plot the
 394 contour lines in the subspace $\varphi_1 \times \varphi_2$ of two objective functions (15) or (17) defined with
 395 two significantly different values of p (for instance, $p = \frac{1}{2}$ and $p = 2$). If the contour lines
 396 of these two objective functions do not intersect, then the parameters can be suspected to
 397 be redundant.

398 Plotting the contour lines of the objective function requires a systematic exploration of
 399 the parameter subspace. An alternative to this approach consists in computing the
 400 dimensionless gradients of the objective functions obtained with two different powers p
 401 and q :

$$402 \quad \mathbf{G}_p = \begin{bmatrix} L_1 \frac{\partial J_p}{\partial \varphi_1} \\ L_2 \frac{\partial J_p}{\partial \varphi_2} \end{bmatrix}, \quad \mathbf{G}_q = \begin{bmatrix} L_1 \frac{\partial J_q}{\partial \varphi_1} \\ L_2 \frac{\partial J_q}{\partial \varphi_2} \end{bmatrix} \quad (22)$$

403 where L_1 and L_2 are scaling factors for the parameters φ_1 and φ_2 (e.g. the typical ranges of
 404 variation of these parameters), and checking colinearity via the dimensionless
 405 determinant

$$406 \quad D = \frac{1}{\|\mathbf{G}_p\| \|\mathbf{G}_q\|} \left(\frac{\partial J_p}{\partial \varphi_1} \frac{\partial J_q}{\partial \varphi_2} - \frac{\partial J_p}{\partial \varphi_2} \frac{\partial J_q}{\partial \varphi_1} \right) \quad (23)$$

407 where the operator $\|\cdot\|$ denotes the norm of the vector. The derivatives of the objective
 408 functions with respect to the parameters may be computed empirically from two values of
 409 J_p and J_q computed using two slightly different values of the parameters. The closer D
 410 to zero, the smaller the angle between the gradient vectors \mathbf{G}_p and \mathbf{G}_q , the more (locally)
 411 redundant the parameters φ_1 and φ_2 .

412 4. Application Example 1: Linear Single Reservoir Model

413 4.1 Governing equations

414 Consider a single reservoir, rainfall-runoff model with a linear discharge law:

$$415 \quad \frac{dU}{dt} = AP(t)c - kU \quad (24a)$$

$$416 \quad U(t_1) = U_1 \geq 0 \quad (24b)$$

417 where A is the catchment area, c is the effective infiltration coefficient, k is the specific
 418 discharge coefficient, $P(t)$ is the precipitation rate, U is the volume of water stored in the
 419 model and kU is the outlet discharge of the model. Note that Eq. (24a) can be written in
 420 the form (8) by defining $g(U, \varphi) = kU$. Classically, A is known and c and/or k must be
 421 calibrated.

422 This model verifies Eqs. (9–11) of assumptions (A1)-(A4), consequently $U(t)$ is
 423 positive for all t .

424
 425 The governing equation for the sensitivity is

$$426 \quad \frac{ds}{dt} = -ks - \frac{\partial(kU)}{\partial\varphi} + \frac{\partial(AcP)}{\partial\varphi} \quad (25a)$$

$$427 \quad s(t_1) = 0 \quad (25b)$$

428

429

Two possibilities arise:

430 (1) The parameter to be calibrated is the effective infiltration coefficient c . In this case,
431 $\varphi = c$ and Eq. (25a) simplifies into

$$432 \quad \frac{ds}{dt} = AP - ks \quad \text{if } \varphi = c \quad (26)$$

433 Eqs. (25a, 26) verify Eqs. (9–11) with $AP > 0$, therefore s is positive for all times.

434

435 (2) The parameter to be calibrated is the discharge coefficient k . In this case, $\varphi = k$ and
436 Eq. (25a) becomes

$$437 \quad \frac{ds}{dt} = -U - ks \quad \text{if } \varphi = k \quad (27)$$

438 Eqs. (25a, 27) verify Eqs. (9–11) with $-U < 0$, therefore s is negative for all times.

439 **4.2 Distance-based objective functions**

440 Assume that a distance-based measure is used for the objective function. If the model
441 is to be calibrated against field measurements (or estimates) of the volume U of water
442 stored in the catchment, then $F(U) = U$ and Eq. (16a) becomes

$$443 \quad \frac{dJ_p}{d\varphi} = bp \int_{\Omega} w |U - V|^{p-2} (U - V) s \, dt \quad (28)$$

444 As shown in the previous subsection, the sign of s is constant over Ω . The particular
445 case of the NSE or SE objective functions, ($p = 2$, $w = 1$) yields the following formula

$$446 \quad \frac{dJ_2}{d\varphi} = 2b \int_{\Omega} (U - V) s \, dt \quad (29)$$

447 Assume now that the model is to be calibrated against the discharge $Q = kU$ at the
448 outlet of the catchment. Then $F(U) = kU$ and $\partial F / \partial U = k$. If the parameter to be
449 calibrated is the coefficient c , then $\varphi = c$ and $\partial F / \partial \varphi = 0$. If the parameter to be
450 calibrated is the discharge coefficient k , then $\varphi = k$ and $\partial F / \partial \varphi = U = Q / k$. Applying
451 Eqs. (16) yields

$$452 \quad \frac{dJ_p}{d\varphi} = bp \int_{\Omega} w |Q - V|^{p-2} (Q - V) ks \, dt \quad \text{if } \varphi = c \quad (30a)$$

$$453 \quad \begin{aligned} \frac{dJ_p}{d\varphi} &= bp \int_{\Omega} w |Q - V|^{p-2} (Q - V) (ks + Q/k) \, dt \\ &= -bp \int_{\Omega} w |Q - V|^{p-2} (Q - V) \frac{ds}{dt} \, dt \quad \text{if } \varphi = k \end{aligned} \quad (30b)$$

454 Note that the second equality in Eq. (30b) is obtained from Eq. (27). Since s is not
455 monotone over Ω in the general case, both $Q - V$ and ds/dt are liable to cancel over Ω and
456 the objective function J_p in Eq. (30b) may have more than one extremum. This is an
457 illustration of Remark (R10). In the particular case of the NSE or SE objective functions
458 ($p = 2$, $w = 1$), the following formulae are obtained

$$459 \quad \frac{dJ_2}{d\varphi} = 2b \int_{\Omega} (Q - V)ks \, dt \quad \text{if } \varphi = c \quad (31a)$$

$$460 \quad \frac{dJ_2}{d\varphi} = 2b \int_{\Omega} (Q - V)(ks + Q/k) \, dt = -2b \int_{\Omega} (Q - V) \frac{ds}{dt} \, dt \quad \text{if } \varphi = k \quad (31b)$$

461 **4.3 Weak form-based objective function**

462 Assume now that the objective function is defined using the weak form-based
463 approach.

464 If the model is to be calibrated against field measurements (or estimates) of the
465 volume of water stored in the catchment, then $F(U) = U$ and Eq. (18) becomes

$$466 \quad \frac{dJ_p}{d\varphi} = bp \int_{\Omega} w |U - V|^p s \, dt \quad (32)$$

467 Since s keeps the same sign over Ω , the derivative of J_p cannot cancel if w is nonzero.
468 Then the points for which $J_p = a$ (a being the optimum value for the objective function)
469 define a line in the parameter space (c, k) . In the particular case ($p = 2, w = 1$), one has

$$470 \quad \frac{dJ_2}{d\varphi} = 2b \int_{\Omega} (U - V)^2 s \, dt \quad (33)$$

471 If the model is to be calibrated using measurements of the outlet discharge $Q = kU$,
472 then $F = kU$, $\partial F / \partial U = k$ and Eqs. (18) gives

$$473 \quad \frac{dJ_p}{d\varphi} = bp \int_{\Omega} w |Q - V|^{p-1} ks \, dt \quad \text{if } \varphi = c \quad (34a)$$

$$474 \quad \begin{aligned} \frac{dJ_p}{d\varphi} &= bp \int_{\Omega} w |Q - V|^{p-1} (ks + Q/k) \, dt \\ &= -bp \int_{\Omega} w |Q - V|^{p-1} \frac{ds}{dt} \, dt \quad \text{if } \varphi = k \end{aligned} \quad (34b)$$

475 An interesting, particular case is that of the Cumulative Error (CE), or Balance Error
476 (BE) indicators (see Appendix A), obtained for ($p = 1, w = 1$):
477

$$478 \quad \frac{dJ_p}{d\varphi} = bA \int_{\Omega} ks \, dt = bAk \int_{\Omega} s \, dt \quad \text{if } \varphi = c \quad (35a)$$

$$479 \quad \frac{dJ_p}{d\varphi} = -b \int_{\Omega} \frac{ds}{dt} \, dt = -b[s(t_2) - s(t_1)] \quad \text{if } \varphi = k \quad (35b)$$

480 Two remarks may be made:

481 (R13) It is visible from Eqs. (32, 34) that the derivative of the weak form-based objective
482 function cannot be zero, except in the trivial case $U = V \, \forall t \in \Omega$. If the objective
483 function is based on the outlet discharge $Q = kU$, the only possibility for its
484 derivative to cancel occurs for $k = 0$, which is meaningful only in the trivial case
485 $kU = V = 0 \, \forall t \in \Omega$.

486 (R14) Comparing Eqs. (35a) and (35b) indicates that the CE and BE indicators are
487 extremely useful in calibrating the runoff coefficient c but are almost useless in
488 calibrating the discharge coefficient k of the conceptual model. This well-known

489 result is confirmed by the following analysis. The ratio of the gradients computed
490 via Eqs. (35a, b) gives

$$491 \quad \frac{dJ_p}{dk} = K \frac{dJ_p}{dc} \quad (36a)$$

$$492 \quad K = \frac{s(t_2) - s(t_1)}{k \int_{\Omega} s \, dt} = \frac{s(t_2) - s(t_1)}{(t_2 - t_1)k \bar{s}} \quad (36b)$$

493 where \bar{s} is the average value of s over Ω . The numerator in K remains bounded. If
494 the input time series is sufficiently long to be assumed stationary, the average value
495 of s does not depend on the length of the time interval $t_2 - t_1$. Consequently the
496 denominator is proportional to the time interval $t_2 - t_1$. Therefore K tends to zero as
497 the length of the calibration interval increases. This means that the CE and BE
498 indicators are insensitive to the value of k when long time series are used.
499 Therefore, they cannot be used to calibrate k when the variable is the outflowing
500 discharge.

501 **4.4 Numerical experiments**

502 The properties of distance- and weak form-based objective functions are investigated
503 using the following numerical experiment. An artificial time series for the observed
504 (measured) variable V is generated using a nonlinear conceptual model with artificially
505 randomized input time series. The water level in the nonlinear reservoir and the
506 outflowing discharge of the nonlinear model are considered as « reality », against which a
507 linear conceptual model is to be fitted. The steps in the generation of the times series are
508 the following.

509 (1) An artificial rainfall time series is generated at a daily time step using the following
510 model:

$$511 \quad P_n = \frac{P_{\max}}{1 - \alpha} \max(\text{Ran} - \alpha, 0) \quad (37)$$

512 where P_{\max} is a constant, Ran is generated randomly from a uniform probability
513 density function between 0 and 1, and α is a threshold value between 0 and 1. Ran
514 is generated every time step independently from the realization at the previous time
515 steps. The probability for a rainfall R_n to be nonzero over a given day n is $1 - \alpha$.

516

517 (2) The generated rainfall signal is used as an input for a nonlinear conceptual model
518 obeying the following equation:

$$519 \quad \frac{dW}{dt} = A(CP - KW^\beta) \quad (38a)$$

$$520 \quad W(0) = 0 \quad (38b)$$

521 where A is the catchment area, C is an infiltration constant, K and β are predefined
522 constants ($\beta \neq 1$) and W is the amount of water stored in the model. Eq. (38a) is
523 solved numerically using an explicit formula at a daily time step:

$$524 \quad W_{n+1} = W_n + A(CP_n - KW_n^\beta) \Delta t \quad (39)$$

525 where P_n is the average value of the rainfall rate between the time levels n and
526 $n + 1$. The explicit approach corresponds to the most widespread implementation of
527 conceptual models available in the literature.
528

529 (3) The numerical solution W_n is used as the observed variable V in the computation of
 530 the objective function. Two possibilities are considered hereafter:

$$531 \quad \left. \begin{array}{l} V = W \\ F(U) = U \end{array} \right\} \quad (40a)$$

$$532 \quad \left. \begin{array}{l} V = AKW^\beta \\ F(U) = AkU \end{array} \right\} \quad (40b)$$

533 Equation (40a) corresponds to the situation where the state variable W can be field-
 534 estimated or measured and where the variable U in the linear model (24a) is
 535 considered to bear a physical meaning. Equations (40b) correspond to the more
 536 widespread calibration technique where the flow variable used in the computation
 537 of the objective function is the discharge at the outlet of the catchment.

538

539 Note that the governing equation (24a) for the linear reservoir model is also solved
 540 numerically using an explicit formula

$$541 \quad U_{n+1} = U_n + A(cP_n - kU_n)\Delta t \quad (41)$$

542 where c and k are the infiltration coefficient and the specific discharge coefficient for the
 543 linear conceptual model. The main motivation behind the choice of a nonlinear
 544 conceptual model to generate the reference time series is that no combination of the
 545 parameters c and k in the linear model (24a) allows the solution W of Eq. (38a) to be
 546 reproduced exactly, which is precisely the case when real-world time series are dealt
 547 with.

548 The parameters used in the present experiment are summarized in Table 1.

549

550 Figure 1 shows the contour lines obtained for two types of distance-based objective
 551 functions. The first objective function $J_{p,U}$ is defined using the amount of water in the
 552 reservoir as in Eqs. (40a):

$$553 \quad J_{p,U} = 1 - \frac{\int_{\Omega} |U - W|^p dt}{\int_{\Omega} |\overline{W} - W|^p dt} \quad (42)$$

554 The second objective function $J_{p,Q}$ is computed from the outflow discharges as in
 555 Eqs. (40b):

$$556 \quad J_{p,Q} = 1 - \frac{\int_{\Omega} |Q - KW^\beta|^p dt}{\int_{\Omega} |\overline{KW^\beta} - KW^\beta|^p dt} \quad (43)$$

557 where the overbar denotes the average over Ω . Eqs. (42-43) are nothing but the
 558 Generalized Nash-Sutcliffe Efficiency (GNSE) presented in Appendix A. In hydrological
 559 modelling, it is more customary to use the discharge as a calibration variable than the
 560 volumes stored in the reservoirs. In Figure 1, the values used for p are $\frac{1}{2}$, 1 and 2.

561

562 Comparing the contour lines obtained using Eq. (42) (Figure 1a, 1c, 1e) and those
 563 obtained using Eq. (43) (Figure 1b, 1d, 1f) illustrates Remark (R11). The objective
 564 functions based on the water depth (or volume) and the objective functions based on the
 565 discharge have radically different contour line shapes. Using two different variables in the
 566 definition of the objective functions brings in more information than using the same

567 variables and changing the value of the power p in the GNSE. Obviously, the optimal
 568 values of the objective functions depend on the variable used in the calibration process
 569 and, to a lesser extent, on the value of the exponent p . Remarks (R9, R10) are illustrated
 570 by the zero contour line in Figure 1d. It is visible from Figure 1d that the derivative
 571 $\partial J_{1/2,Q} / \partial k$ cancels for small values of k around $c = 1.0$. This corresponds to the change
 572 in curvature of the zero contour line next to the c -axis. The objective function is not
 573 monotone with respect to k in this region of the parameter space. In the present case,
 574 however, this is not too serious a problem because (i) the extremum corresponds to a
 575 minimum in the objective function, and (ii) it is located far away from the maximum of
 576 the objective function. However, in the general case, this is a potential source for local
 577 extrema in the objective function.

578
 579 Figure 2 shows the contour lines obtained for two types of weak form-based objective
 580 functions. The first objective function $J_{p,U}$ is defined using the state variables U and W as
 581 in Eqs. (40a):

$$582 \quad J_{p,U} = \frac{\int_{\Omega} |U - W|^{p-1} (U - W) dt}{\int_{\Omega} |\overline{W} - W|^p dt} \quad (44)$$

583 The second objective function $J_{p,Q}$ is computed from the outflow discharges as in
 584 Eqs. (40b):

$$585 \quad J_{p,Q} = \frac{\int_{\Omega} |Q - KW^{\beta}|^{p-1} (Q - KW^{\beta}) dt}{\int_{\Omega} |\overline{KW^{\beta}} - KW^{\beta}|^p dt} \quad (45)$$

586 where the overbar denotes the average over Ω . Note that the denominator in Eqs. (44, 45)
 587 is similar to that in Eqs. (42, 43) and therefore the scaling is the same. In contrast with
 588 Eqs. (42, 43), the best model fit is achieved for $J_{p,U} = 0$ and $J_{p,Q} = 0$. Also note that for
 589 $p = 1$ (Figure 2d), Eq. (45) gives an information similar to the Cumulative Error (CE) or
 590 Balance Error (BE).

591
 592 Remarks (R9, R10) are illustrated by the zero contour line in Figure 2b. Indeed, the
 593 derivative $\partial J_{1/2,Q} / \partial k$ cancels for ($k = 0.15$, $c = 0.2$). This corresponds to the curved
 594 contour in the bottom right corner of the Figure. The objective function is not monotone
 595 with respect to k in this region of the parameter space.

596 As in the case of the distance-based objective functions (42, 43), comparing Figures
 597 2a, 2c, 2e and Figures 2b, 2d, 2f illustrates Remark (R11) on the complementary
 598 character of the information brought by objective functions defined using different model
 599 variables. However, contrary to distance-based objective functions, it is possible to find
 600 parameter combinations for which the objective functions defined by both equations (44)
 601 and (45) are optimal.

602 Remark (R13) on the strictly monotone character of the weak form-based objective
 603 functions is also confirmed.

604 Figure 2d confirms Remark (R14) that the specific discharge coefficient k cannot be
 605 calibrated using CE or BE because the CE and BE indicators have identical values for all
 606 k . At the same time, the CE or BE indicators are extremely useful in calibrating the
 607 infiltration coefficient because there is only one possible value of c for which $J_{1,Q} = 0$.

608 Moreover, the intersection of all the zero contour lines in Figure 2 are very close to the
 609 optimum values for the distance-based objective functions using the discharge as a

610 calibration variable (Figure 1b, 1d, 1f). This indicates that the set of distance-based
 611 objective functions may yield a calibration result close to that given by the commonly
 612 admitted distance-based approach, while eliminating the local extremum problem
 613 associated with distance-based objective functions.

614 This example also illustrates the fact that optimum values obtained from distance-
 615 based functions are often mutually exclusive, which is not the case with weak form-based
 616 functions.

617 5. Application Example 2: a Multiple Reservoir Model with Threshold Function

618 5.1 Model presentation

619 The Medor model (Hreiche et al., 2003) is a three-reservoir model (Figure 3) initially
 620 designed for hydrological modelling over arid or semi-arid regions. A variation of this
 621 model has been applied recently to the modelling of karst catchments in the
 622 Mediterranean area (Fleury, 2005; Tritz et al., 2010). The top reservoir accounts for
 623 production. The input to this reservoir is the precipitation rate P , the outputs are the
 624 evapotranspiration rate E and the net precipitation rate I . E may be set equal to the
 625 potential rate, computed from standard evapotranspiration formulae (Fleury, 2005), or
 626 interpolated from monthly data (Tritz et al., 2010). E is limited only when the reservoir is
 627 empty ($H = 0$) and precipitations are insufficient ($P < E$). I is zero until the water level H
 628 in the production reservoir reaches the maximum value H_{\max} . In such a case, the net input
 629 $P - E$ is transferred instantaneously to the other two reservoirs. From a conceptual point
 630 of view, the production reservoir represents the soil layer, from which previously
 631 precipitated water may be restituted to the atmosphere via evapotranspiration. Note that
 632 when the soil reservoir is empty, it remains so until $P - E$ becomes positive again.

633 The net precipitation is routed to a fast response and a slow response reservoir via a
 634 distribution coefficient x , $0 \leq x \leq 1$. Each of these two reservoirs obeys a linear discharge
 635 law. The output hydrograph is the sum of the output discharges from the fast and slow
 636 reservoir. From a physical point of view, the two reservoirs may account for different
 637 flow routing paths over the catchment. From the point of view of the transfer function of
 638 the model, such a structure allows both the rapid recession part of hydrographs and the
 639 slower fluctuations of the base flow to be accounted for via linear laws.

640
 641 The governing balance equations are the following:

$$642 \quad \frac{dH}{dt} = \begin{cases} P - E - I & \text{if } H > 0 \\ 0 & \text{if } H = 0 \text{ and } P - E < 0 \end{cases} \quad (46a)$$

$$643 \quad \frac{dH_1}{dt} = xI - \frac{Q_1}{A} \quad (46a)$$

$$644 \quad \frac{dH_2}{dt} = (1-x)I - \frac{Q_2}{A} \quad (46c)$$

645 where H_1 and H_2 are respectively the water levels in the fast and slow reservoirs. I , Q_1
 646 and Q_2 are given by

$$647 \quad I = \begin{cases} 0 & \text{if } H < H_{\max} \\ P - E & \text{if } H = H_{\max} \end{cases} \quad (47a)$$

$$648 \quad Q_1 = Ak_1H_1 \quad (47b)$$

$$649 \quad Q_2 = Ak_2H_2 \quad (47b)$$

650 where k_1 and k_2 are the specific discharge coefficients of the two reservoirs. The total
651 outflowing discharge is computed as the sum of Q_1 and Q_2 .

652 **5.2 Principle of the parameter redundancy test**

653 It is first noticed that the total amount of water flowing to the outlets of the reservoirs
654 is strongly conditioned by the maximum water level H_{\max} in the production reservoir.
655 Indeed, I is nonzero only when H reaches H_{\max} . The larger H_{\max} , the smaller the time
656 during which I is nonzero, the smaller the amount of water flowing to the reservoirs H_1
657 and H_2 .

658 Consider now the configuration of the model where the specific discharge coefficient
659 of one of the two reservoirs (say, k_2) is zero. In this case, the water may accumulate
660 indefinitely in this reservoir, while the outflowing discharge from this reservoir remains
661 zero. In other words, if $k_2 = 0$, the reservoir H_2 acts as a loss and only a fraction xI of the
662 total infiltration rates participates to the outflow. Therefore, x also controls the outflowing
663 discharge to some extent.

664 Clearly, H_{\max} and x exert a similar influence on the outflowing discharge when $k_2 = 0$.
665 In other words, they are redundant with respect to total discharge, for $k_2 = 0$.
666 Consequently, plotting two different objective functions (18a-b) with two different values
667 of p in the parameter space (H_{\max}, x) should yield non-intersecting contour lines for the
668 two objective functions.

669 **5.3 Catchment and modelling data**

670 The Medor model was used to simulate daily discharge at the outlet of the Bani
671 catchment (Figure 4). This large west-African catchment is characterized by a monsoon
672 climate with a strong north-south rainfall gradient, and considerable rainfall variability
673 since the mid-20th century. As a result, the flow at the Douna gauging station (Figure 4)
674 fell by 68% from 1952–1970 to 1971–2000, with a decrease in the deep water recharge
675 and in base runoff contribution to the annual flood (Ruelland et al., 2009). Some of the
676 low-water periods were severe to the point that river flow at Douna stopped at times
677 during the 1980s.

678 The Medor model may seem too simple at first sight for an operation at a daily time
679 step given the dimensions of the catchment and the time scale of the discharge signal.
680 However, experiments carried out using models of varying complexity have shown that
681 complex transfer functions involving signal delay (such as the unit hydrograph
682 convolution approach) do not contribute to improve model performance significantly
683 (Ruelland et al., 2010). In a similar fashion, using spatially distributed rainfall inputs and
684 model parameters was not seen to improve the quality of the simulated hydrographs
685 significantly. The inertia of the linear reservoirs in the Medor model are seen to be
686 sufficient to model the rainfall-discharge transformation in a satisfactory way. This
687 simpler model is thus retained for the analysis.

688 The model was applied to the 1967–1985 period, for which the discharge record was
689 continuous at the Douna station. Daily rain series were derived from 72 rain gauges
690 covering the area (Figure 4). An average of 70 gauges (with a minimum of 66) were used
691 to interpolate daily rainfall maps by the inverse distance method, which proved to
692 perform best (Ruelland et al., 2008). Potential evapotranspiration forcing consisted of
693 monthly maps produced by the Climatic Research Unit (University of East Anglia, UK)
694 from ~100 stations spread over West Africa, using Penman's method and spline
695 interpolation (New et al., 2000). Since potential evapotranspiration varies slowly over the
696 year, monthly data were disaggregated evenly to the daily time step within each month.
697 The first five years of simulation were used as model warm-up, to eliminate the influence
698 of initial conditions. This five year period was determined from the order of magnitude of
699 the specific discharge coefficients in the model. Indeed, as shown in Appendix B (section

700 B.3), a model with a specific discharge coefficient k requires a warm-up period of at least
 701 a few times $1/k$ for the influence of initial conditions to be eliminated. The parameters
 702 used in the experiment are given in Table 2. The catchment area A is known from
 703 previous studies (Ruelland et al., 2008), while the specific discharge coefficient k_1 is
 704 taken equal to the value that allows the NSE index to be maximized.

705 **5.4 Redundancy test results**

706 Figure 5 shows the contour lines obtained for the distance-based and weak form-based
 707 objective functions. The powers used in Eqs. (43) and (45) are $p = 1/2$ and $p = 2$.
 708

709 Figure 5e is a superimposition of Figures 5a and 5c, while Figure 5f results from the
 710 superimposition of Figures 5b and 5d. In Figures 5e-f, the dashed and solid lines are
 711 respectively the contour lines of the objective functions for $p = 1/2$ and $p = 2$. Except in the
 712 upper left part of the diagram, the contour lines do not intersect, which confirms that the
 713 parameters H_{\max} and x become redundant over most of the parameter space when $k_1 = 0$ or
 714 $k_2 = 0$.

715 **6. Conclusions**

716 Model performance assessment and objective functions classically used in
 717 hydrological modelling may be classified into distance-based and weak form-based
 718 objective functions.
 719

720 Distance-based objective functions have the advantage that the calibration problem is
 721 transformed into a straightforward, single-criterion optimization problem. Their drawback
 722 is the possible appearance of local extrema in the response surface of the model, thus
 723 triggering the failure of classical gradient-based methods and requiring the use of more
 724 computationally demanding global optimization algorithms.

725 Weak form-based objective functions transform the calibration exercise into a root
 726 finding problem.
 727

728 The theoretical considerations in Sections 2-3 and the application examples in
 729 Sections 4-5 lead to the following conclusions.

730 (C1) Weak form-based objective functions are more monotone than distance-based
 731 objective functions when applied to conceptual hydrological models. Monotony
 732 can be proved mathematically for models verifying Assumptions (A1–4) in
 733 Subsection 3.1.

734 (C2) The subset of zero values of weak form-based objective functions form
 735 hypersurfaces in the parameter space. A model with N parameters can be calibrated
 736 by defining N weak form-based objective functions and finding the intersection of
 737 the corresponding N hypersurfaces in the parameter space. Since the weak form-
 738 based objective functions are monotone, the intersection is unique. This allows
 739 classical gradient-based algorithms to be used without the need for more
 740 sophisticated optimum search techniques. The N different objective functions may
 741 be defined by using (i) different observation variables, (ii) transformations of these
 742 variables, (iii) different values for the power p used in the formulation of the weak
 743 form-based function (see equation (7)). Note that the need for a number of
 744 independent criteria matching the number of parameters to be calibrated was
 745 already pointed out by Gupta et al. (2008).

746 (C3) In contrast, distance-based objective functions yield mutually exclusive optimal
 747 parameter sets when different calibration variables are used. Using weak form-

- 748 based objective functions allows this drawback to be eliminated. This allows for
749 multi-objective calibration without the inconvenience of multiple solutions.
- 750 (C4) Distance-based objective functions being widely recognized in the field of
751 hydrological modelling, they could also be used in combination with weak form-
752 based objective functions in the framework of multi-criteria optimization
753 algorithms. A typical multicriteria optimization problem may then consist in
754 maximizing the distance-based objective function under the constraint that all the
755 weak form-based objective functions are zero.
- 756 (C5) Using the same type of objective function (distance-based, see Eqs. (48) or weak
757 form-based, see Eqs. (49)) with two different values of p yields two families of
758 contour surfaces in the parameter space. Non-intersecting families of contour
759 surfaces in the parameter space indicate redundancy between two or more
760 parameters.
- 761 (C6) The theoretical analysis in Section 3 and the application example in Section 4 show
762 that using the volume stored in the reservoir as a calibration variable for the
763 discharge coefficient may be more appropriate than using the discharge.
764 Conversely, the outlet discharge may be a more appropriate variable to calibrate an
765 infiltration (or net rainfall) coefficient via a weak form-based objective function.
- 766 (C7) Assuming that weak form-based objective functions are to be used, the calibration
767 problem is best posed when the hypersurfaces as defined in (C2) are as orthogonal
768 to each other as possible. Therefore, it is advisable to define such objective
769 functions using as many different model state variables as possible (e.g. discharges
770 between various reservoirs in the model, volumes stored in the various reservoirs,
771 etc.).
- 772 (C8) A necessary condition for (C5-6) to be applicable, however, is that the internal
773 variables and fluxes in the model bear a physical reality and be field-measurable.
774 Due to hydrological/hydraulic variability, translating field measurements (e.g. of
775 soil moisture, or piezometric head in aquifers) into variations of model internal
776 variables is not an easy task. This most probably calls for the definition of a
777 different kind of objective functions. For instance, the trends (rising or falling;
778 increasing or decreasing) of the measured and model internal variables over certain
779 periods may be used in the form of indicators. Note that internal variables may not
780 necessarily be useful only to the calibration of a model. Even if not incorporated
781 into the objective function, they may be used to discriminate between different
782 models (or different parameter sets within the same model) giving similar values of
783 objective functions computed from the outflowing fluxes.
- 784 (C9) The result of the calibration/validation process may be biased if the model has not
785 been run over a sufficiently long warm-up period for the influence of possibly
786 inaccurate initial conditions to be eliminated (see section B.2 in Appendix B). The
787 minimum length of the warm-up period is a function of the parameters of the
788 model. Consequently, it should not only be defined a priori: an a posteriori check is
789 needed once the model has been calibrated.

791 The theoretical considerations presented in this paper are valid for hydrological
792 models obeying first-order differential equations. Whether such conclusions also hold for
793 models involving delay functions (e.g. the GR3J model (Edijatno et al., 1999) that
794 embeds a unit hydrograph transformation) or other functions not verifying exactly the
795 governing assumptions in Section 3 is the subject of ongoing research. Future research
796 should also focus on (i) the robustness of weak form-based objective functions compared
797 to the well-established distance-based approach and (ii) the effects of data uncertainty on
798 the behaviour of the objective function. Although only conceptual models were

799 considered in this study, the approach might be applicable to the calibration of some
800 physically-based hydrological models, e.g. when backwater effects are insignificant,
801 however such extrapolation should be subject to further theoretical investigation.

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805

806

807 **Appendix A. Classical Objective Functions**

808 The functions are classified in Table A.1 into to Distance-based (D) and Weak form-
 809 based (W) objective functions. a , b and p in Table A.1 are respectively the offset
 810 constant, the scaling constant and the power used in equations (4) and (7).

811

812 (Table A.1 here)

813 **Appendix B. Proofs**814 **B.1 Sign of the solution U of Eq. (8)**

815 Assume that Eq. (8) holds, with assumptions (A1-4) verified. From Assumption (A3),
 816 at any time t there exists $U_0(t) > 0$ such that $dU/dt = 0$ for $U = U_0$. U_0 verifies Eq. (11),
 817 that is:

$$818 \quad g(U_0, \varphi) = R(U_0, \varphi, t) \quad (\text{B.1})$$

819 If $U(t)$ is smaller than U_0 , then $dU/dt = R - g$ is positive because of Assumption (A2),
 820 and U can only increase at time t . Hence, $U(t)$ is either greater than U_0 or increasing, and
 821 thus can never be negative for $t > t_1$ since $U(t_1) \geq 0$ (Assumption (A4)).

822

823 **B.2 Sign of the sensitivity s in Eqs. (13)**

824 The sensitivity equations (13) are rewritten as

$$825 \quad \frac{ds}{dt} = \alpha s + \beta \quad (\text{B.2a})$$

$$826 \quad \alpha = \frac{\partial}{\partial U} (R - g) \quad (\text{B.2b})$$

$$827 \quad \beta = \frac{\partial}{\partial \varphi} (R - g) \quad (\text{B.2c})$$

$$828 \quad s(t_1) = 0 \quad (\text{B.2d})$$

829 From assumption (A2), α is negative and β has a constant sign. The case $\beta = 0$ leads
 830 to the trivial solution $s = 0$ and is not considered hereafter.

831

832 Consider first the case $\beta > 0$. In this case, there exists an equilibrium value $s_0 = -\beta / \alpha$
 833 for the sensitivity, with $ds/dt = 0$ for $s = s_0$ in Eq. (B.2a). Since α is negative and β is
 834 positive, s_0 is always positive. If $s < s_0$, $ds/dt = \alpha s + \beta > 0$. Hence, s is either larger than
 835 the positive value s_0 or increasing. Since $s(t_1) = 0$ (Eq. (13b)), $ds/dt > 0$ at $t = t_1$ and
 836 $s(t) > 0$ for all $t > t_1$.

837

838 Reasoning by symmetry leads to the conclusion that $s(t) < 0$ for all $t > t_1$ when $\beta < 0$.839 **B.3 Sensitivity to initial conditions and model warm-up period**

840 The purpose is to study the sensitivity of model output to the initial conditions.
 841 Consider the linear model

$$842 \quad R = P - ET \quad (\text{B.3a})$$

$$843 \quad g = -kU \quad (B.3b)$$

844 If the purpose is to study the influence of initial conditions, the parameter φ is $\varphi = U_0$

845 In this case, α and β in equation (B.2a) are given by

$$846 \quad \alpha = -k \quad (B.4a)$$

$$847 \quad \beta = 0 \quad (B.5a)$$

848 Considering that the sensitivity of U with respect to the initial condition is equal to 1
849 for $t = 0$, the solution of equations (B.2a, B.4a, B.4b) is a decreasing exponential:

$$850 \quad s(t) = \exp(-kt) \quad (B.6)$$

851 The sensitivity of U (and therefore of any function $F(U)$) becomes negligible after a
852 simulation period equal to a few times $1/k$. The warm-up period, that is necessary to
853 eliminate the influence of a possible wrongly defined initial condition, should therefore
854 be taken equal to a few times $1/k$. For instance, $s(3/k) = 4.98\%$; $s(4/k) = 1.8\%$ and
855 $s(5/k) = 0.7\%$. In other words, only 0.7% of the initial sensitivity to the initial conditions
856 remains after a simulation period $5/k$.

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