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KarstMod: a modelling platform for rainfall - discharge analysis and modelling dedicated to karst systems

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Abstract

We propose an adjustable modelling platform (KarstMod) for both the simulation of spring discharge at karst outlets and analysis of the hydrodynamics of the compartments considered in the model. KarstMod provides a modular, user-friendly modelling environment for educational, research and operational purposes. It can reproduce the structure of most conceptual lumped models of karst systems in the literature. The modularity of the platform allows to compare different hydrosystems within the same methodological approach. To promote good modelling practices, the platform provides a variety of graphs and tools that facilitate improved understanding and insights in the behaviour of the models, and that detect possible flaws in structure and parameterization. The model and users manual are freely downloadable from the SNO Karst website (www.sokarst.org)

Keywords: Data visualization, hydrology, hydrogeology, sensitivity analysis, modelling, Environmental Decision Support Tool

Software availability

Name of software	KarstMod
Description	KarstMod is a collaborative project developed by the French SNO Karst. It provides an adjustable modelling platform for both the spring discharge simulation at karst outlets and hydrodynamic analysis of the compartments considered in the model.
Developers	N. Mazzilli and D. Bertin
Availability	Free to the public (contact the developers)
Contact address	karstmod@services.cnrs.fr
Year first available	2014
Software required	Java Runtime Environment 1.8
Program language	Java
Package size	2.8 Mo
Availability	http://www.sokarst.org/
Current version	1.5.5
Cost	free of charge

Introduction

Karst has been defined as “the medium where heterogeneity reaches its paroxysm” [18]. Indeed, high porosity and thus high permeability contrasts are typical of karst aquifers. These contrasts result in a duality of infiltration (either diffuse or concentrated) and of flow regimes (either laminar or turbulent). The karstification process itself, its self-organization ability [33] and the rapid evolution of karst conduits result in highly non-linear hydraulic connexions within, and global functioning of karst aquifers. With increasing demand for water, karst aquifers have grown more important as a resource. Modelling the rainfall - discharge relationship is an essential step in estimating the sustainable yield of karst aquifers but also in predicting the impacts of climatic or anthropogenic forcing on groundwater resources in the long term. Even so, characterization and modelling of karst aquifers remains a challenging task. Among the different modelling approaches,

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lumped modelling is recognised as a major tool for analyzing hydrological processes and for managing water resource. These models are based on physically sound structures and equations selected by the modeler as representative of the main processes involved, together with semi-empirical processes [1]. This approach is particularly well suited to karst environments where knowledge of system geometry is usually difficult to gather [8, 12].

The parameters of lumped models cannot be determined directly from physical catchment characteristics, and thus parameter values must be estimated by calibration against observed data. The structure of compartment models is thus a trade-off between adaptability (the model must be able to represent a large variety of hydrological conditions) and parsimony (parameters must be identifiable and over-fitting must be prevented) [23]. Effective model development practices include careful sensitivity analysis and uncertainty assessment, to assess model performance and also model uncertainty and physical realism [32, 26]. An overview of sensitivity analysis and its link to model calibration and evaluation is provided in [25].

In this paper, we propose an adjustable modelling platform (KarstMod) for both the spring discharge simulation at karst outlets and hydrodynamic analysis of the compartments considered in the model. KarstMod provides a modular, user-friendly modelling environment for educational, research and operational purposes. It can reproduce the structure of conceptual lumped models of karst systems in the literature. The modularity of the platform allows a comparison of different hydrosystems through a single methodological approach. To promote valid modelling practices, the platform provides a variety of graphs and tools that facilitate improved understanding and insight into the behaviour of the models, and that detect possible flaws in structure and parameterization. Section 1 is a description of the platform. Section 2 illustrates KarstMod functionalities based on model application to the Fontaine de Vaucluse site of the SNO Karst network.

1. Platform overview

1.1. Workflow

In the first step, the user defines the model structure and fluxes using the graphical interface. As stated in the introduction, lumped models are based on physically sound structures and equations. The user may thus use his understanding of the main processes involved to define the model. However, we recommend a gradual complexification approach, with careful assessment of the influence of the selected compartment and fluxes on the resulting model behaviour and equifinality. The next step is to specify user-defined values of rainfall (P), evapotranspiration (ET) and reservoir pumping. The user also defines the performance measure and the warm-up, calibration and validation periods.

The model can run using user-specified parameter values ("run mode"), or in an automatic calibration mode. Most model outputs are available in both run and calibration modes (Fig. 1). The run mode may be especially useful for educational and learning purposes because it allows a direct analysis of the effect of the model parameters on the model results. Manual calibration may also leave the users (e.g. students) facing non-linearity of the model response. Calibration mode provides a systematic exploration of the parameters space. The outcomes of this exploration are the selection of the optimal parameter set for a selected performance measure, and a set of graphs that allow a first grasp of equifinality issues (see Section 1.4.2).

1.2. Model structure and equations

Karst aquifers can be consensually decomposed into an infiltration and a saturated zone [24, 29] :

- the infiltration zone comprises the soil and epikarst subsystem, which may store part of the infiltrated water, plus the unsaturated subsystem, which connects the epikarst to the phreatic zone by drainage through a vertical network of fissures and conduits. It may be locally saturated.
- the saturated sub-system is split into a network of high permeability conduits and low permeability volumes with a high storage capacity.

The relative importance of these compartments in the hydrological functioning of the karst system depends on rock texture and structure and on the karst aquifer genesis history. Non-linearity affects the hydraulic connexions within and between the different compartments [15].

The modular structure proposed in KarstMod is based on this conceptual model, a thorough literature review of existing lumped models, and consideration of equifinality issues. In its most complete form, the platform offers 4 compartments organized on as a two-levels structure (Figure 2): (i) compartment E (higher level), (ii) compartments L, M and C (lower level). A priori, the higher level stands for the infiltration zone, and the lower level stands for the saturated zone where the compartments L, M, C stand for the different sub-systems of the saturated zone. However the user is free to assign model compartments to different conceptual model. In compartment E, the minimum water level can be either zero or lower (soil-available water content configuration, see Figure 2). To complement linear and non-linear water level - discharge laws which are traditionally used in lumped models, KarstMod proposes (i) an hysteretic discharge - water level function which is meant to reproduce hysteretic dependence observed on wet-dry cycles in the vadose zone [16, 31], (ii) a exchange function proportional to the water level difference between two compartments, which is meant to reproduce matrix-conduit interactions as supported by direct observations of a variety of karst systems (e.g. [14, 2, 19]). The model nomenclature is detailed in appendix.

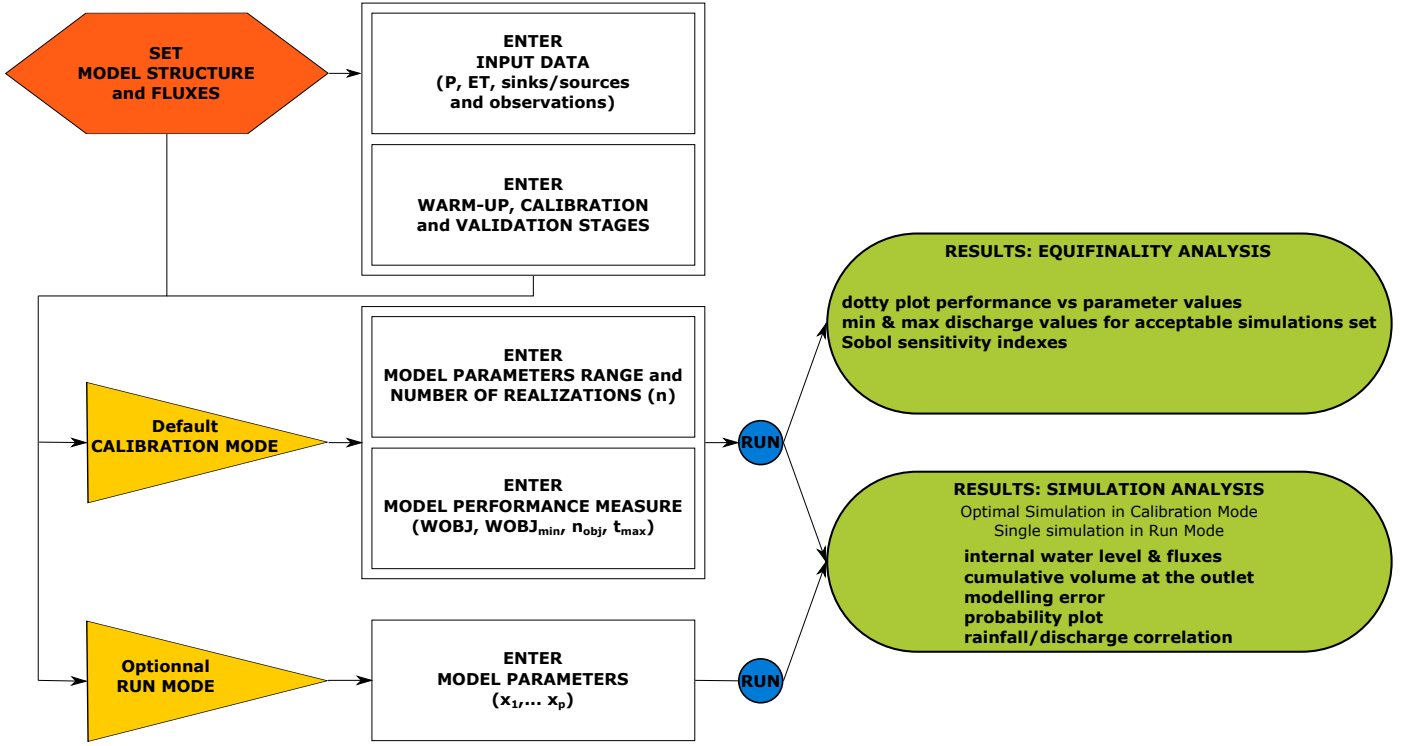


Figure 1: Synthetic workflow for the KarstMod platform. Hexagon, triangles, rectangles, circles and ellipsoids represent respectively building step on graphical interface, choice of simulation mode, input data and parameters, calculation step and results. Abbreviations are detailed in appendix 3.

The model has 5 balance equations:

$$\frac{dE}{dt} = P - ET - Q_{loss} - Q_{EL} - Q_{EM} - Q_{ES} - Q_{EC} - Q_{hyEC} - Q_{hyES} \quad \text{if } E \geq 0 \quad (1a)$$

$$\frac{dE}{dt} = P - ET \quad \text{if } E_{min} < E < 0 \quad (1b)$$

$$\frac{dL}{dt} = Q_{EL} - Q_{LS} - Q_{pump}^L \quad (1c)$$

$$\frac{dM}{dt} = Q_{EM} - Q_{MC} - Q_{MS} - Q_{pump}^M \quad (1d)$$

$$\frac{dC}{dt} = Q_{EC} + Q_{hyEC} + Q_{MC} - Q_{CS} - Q_{pump}^C \quad (1e)$$

where:

- E, L, M and C [L] are the water levels in the compartments E, L, M and C respectively,
- E_{min} [L] is the minimum water level in compartment E,
- P [L/T] is the precipitation rate,
- ET [L/T] is the evapotranspiration rate,
- Q_{pump}^L, Q_{pump}^M and Q_{pump}^C [L/T] are the discharge rates removed from compartment L, M and C respectively, per unit surface area,
- $Q_{loss}, Q_{EM}, Q_{ES}, Q_{EC}, Q_{hyEC}, Q_{hyES}, Q_{LS}, Q_{MS}, Q_{CS}, Q_{MC}$ [L/T] are internal discharge rates per unit surface area.

The discharge at outlet Q_S is given by:

$$Q_S = R_A \times (Q_{ES} + Q_{LS} + Q_{MS} + Q_{CS} + Q_{hyES}) - Q_{pump}^S \quad (2)$$

where R_A [L²] is the recharge area of the catchment and Q_{pump}^S [L/T] is the discharge rate removed at the outlet per unit surface area. The internal fluxes are detailed in the user's guide.

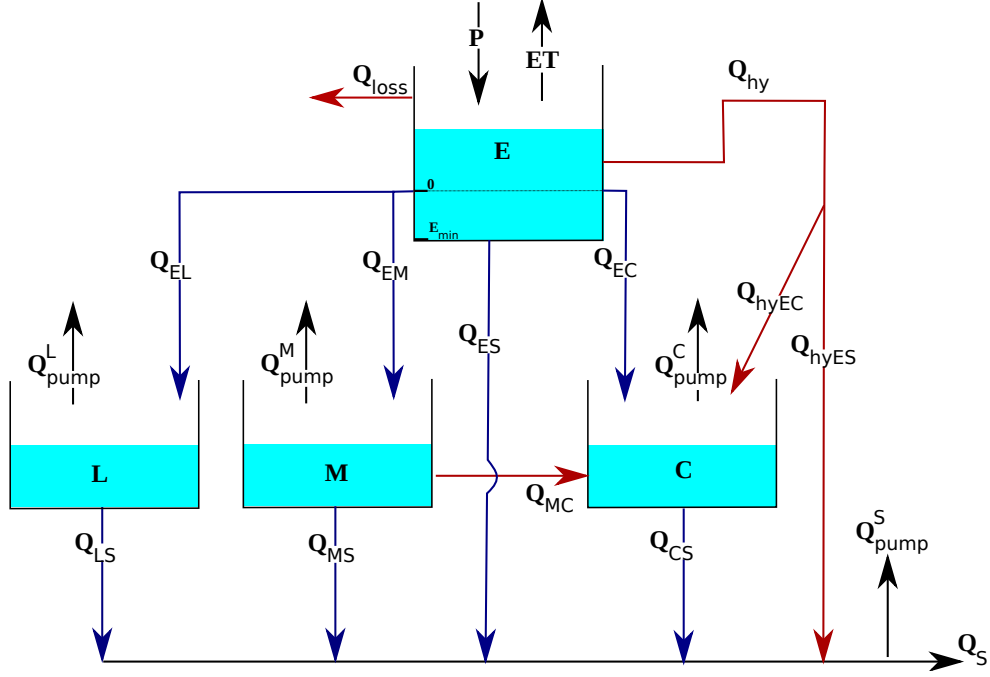


Figure 2: Structure of the modular platform. In this view all compartments and fluxes are activated, the minimum water level of $E_{min} < 0$ is set for compartment E, and the hysteretic function is used.

1.3. Model calibration

Warm-up, calibration and validation periods are controlled entirely by the user. The model provides the possibility to calibrate the initial water level in the activated compartments. Discontinuous calibration and validation periods are allowed.

The performance criteria proposed in KarstMod are the Nash-Sutcliffe efficiency NSE [22] and the modified Balance Error BE [23]. The user may apply the performance criteria to either the full range of the variable or to values above or below discharge thresholds. These functionalities make it possible to limit the influence of high discharge values in the NSE and to focus the analysis on either high or low flow periods.

KarstMod allows either single or multi-objective calibration approaches. The objective function used in the calibration procedure is either one of the performance criteria defined above, or an aggregated objective function defined as the weighted sum of two performance criteria. In the following, we use WOBJ as a generic notation for the selected objective function. The multi-objective problem is thus reduced to a scalarized one.

The model is calibrated using a quasi Monte-Carlo procedure, with a Sobol sequence sampling of the parameter space [30]. The procedure is stopped when either n_{max} parameter sets satisfying WOBJ greater than the user-defined threshold value $WOBJ_{min}$ are collected, or when the elapsed simulation time reaches the maximum duration t_{max} specified by the user. The user specifies both $WOBJ_{min}$ and t_{max} .

The differential model equations 1 are solved using a fourth-order Runge-Kutta scheme and user-specified initial water levels in the selected compartments as initial conditions.

1.4. Model outputs

1.4.1. Optimal simulation analysis

The optimal parameter set is defined as the parameter set of the Sobol sequence sampling that yields the best model performance over the calibration period, with respect to the objective function WOBJ. The optimal simulation is the simulation that results from a model run, using the optimal parameter set. Regarding the optimal simulation, the following graphs are available : (i) internal and external variables and fluxes as a function of time, (ii) cumulative volumes at the outlet as a function of time, (iii) simulated mass balance per time step, (iv) simulation error as a function of time, (v) Q_S versus Q_{obs} plot. These graphs make it possible to investigate the internal behaviour of the model and to detect possible drifts. The Q_S versus Q_{obs} plot highlights simulation error variability during the simulation period. The following analyses are also available : (i) cumulative probability plots for the (Q_S) and observed (Q_{obs}) discharges, (ii) auto-correlogram of P , (iii) cross-correlogram between P and Q_S , P and Q_{obs} , Q_{obs} and Q_S . The discharge cumulative probability plots provide insight into processes that may influence the distribution law of discharge values, such as the existence of overflow springs, or the extra input or output of water coming from or towards a neighbouring system [17, 20]. The simple and cross spectral analyses complete the study of correlogram functions providing information on the regulation time of the system, i.e. its inertia related to the nature of its storage and on the frequency of the phenomena that produce flow variations at the spring [17].

1.4.2. Equifinality analysis

Most environmental problems are ill-posed i.e. encounter issues about the unicity, identifiability and stability of the problem solution [6]. As a consequence, many different representations of the modelled system may be considered as

equally acceptable [4]. In KarstMod, parametric equifinality can be investigated using the following tools:

- dotted plots of the values of the objective function (calibration period) against the values of the parameters X_i , for all the parameter sets of the Sobol sequence that satisfy $WOBJ > WOBJ_{min}$. These plots provide a preliminary analysis of the distribution of the optimum values of each parameter.
- dotted plot of the values of the performance criteria used to define the aggregated objective function, for all the parameter sets of the Sobol sequence that satisfy $WOBJ > WOBJ_{min}$. These plots allow to investigate possible conflicts between the performance criteria (Pareto frontier) [11].
- variance-based, first-order S_i and total S_{Ti} sensitivity indexes for the model parameters X_i . These indexes help estimating the influence of the parameters on the model output, and thus to detect over-parameterization.

The sensitivity indexes are related to the decomposition of the variance of the calibration variable (here, the discharge at the outlet) into terms either due to each parameter i taken singularly (first order indices), or to the interactions between parameters [27]. Both indexes are calculated using the Sobol procedure described in [28].

KarstMod enables to use the simulation results from all parameter sets yielding $WOBJ > WOBJ_{min}$ for the evaluation of the uncertainty on the simulation results. The approach is derived from the Regional Sensitivity Analysis (RSA) [13] and the Generalized Likelihood Uncertainty Estimation (GLUE) [3]. Instead of selecting a unique parameter set as the outcome of the calibration process, these methods consider that all parameter sets yielding satisfactory results over the calibration period (behavioural parameter sets) should be considered in the prediction process. The value of $WOBJ$ over the calibration period is used as a likelihood measure for each behavioural parameter set. Based on this assumption, KarstMod produces the following simulation results:

- minimal and maximal discharge values simulated at time t from the behavioural parameter sets. They help figure out the spread of the simulation results for the behavioural parameter sets.
- limits for the 90% confidence interval for the simulated discharge at time t .
- the most likely value of the simulated discharge, which is estimated considering both the objective function and the threshold value defined by the user to constrain the behavioural parameters set.

2. Test Case

The fontaine de Vaucluse spring is the only outlet of a 1115 km² recharge area located South-East of France. Its mean flow rate is one of the highest in Europe (18 m³ over the 1966-2016 period). A 3-compartments lumped model of the rainfall-discharge relationship was proposed by Fleury et al [7]. The upper, soil compartment feeds two lower compartments that respectively simulate rapid and slow discharges. The authors used rainfall and temperature time series from four weather gauging stations to derive the meteorological P and ET inputs. Calibration was performed using the 1995-1996 hydrological year with no warm-up period, based on the Nash-Sutcliffe efficiency. We have been able to successfully reproduce the model structure (see Figure 3) and results from [7] using KarstMod. The platform also allows to test the sensitivity to the initial conditions. We let all parameters vary across a one order of magnitude range. Initial water levels were also allowed to vary. The calibration range for the initial water levels has been set according to the observed water levels range during simulation. We ran the calibration with no warm-up period and with a one-year warm-up. Figure 4 shows the observed and simulated discharge, with the confidence interval for the simulated discharge. Figure 5 shows the sensitivity indexes. When no warm-up is used, the sensitivity to the initial conditions may be greater than the sensitivity to model parameter k_{EC} which suggests that the calibration result is sensitive to the initial water levels. Using a one-year warm-up, the spread of the simulated discharge reduces in the first months of the calibration. The effect of the initial conditions on the calibration results becomes negligible as compared to the effect of the model parameters, as evidenced by the new sensitivity indexes.

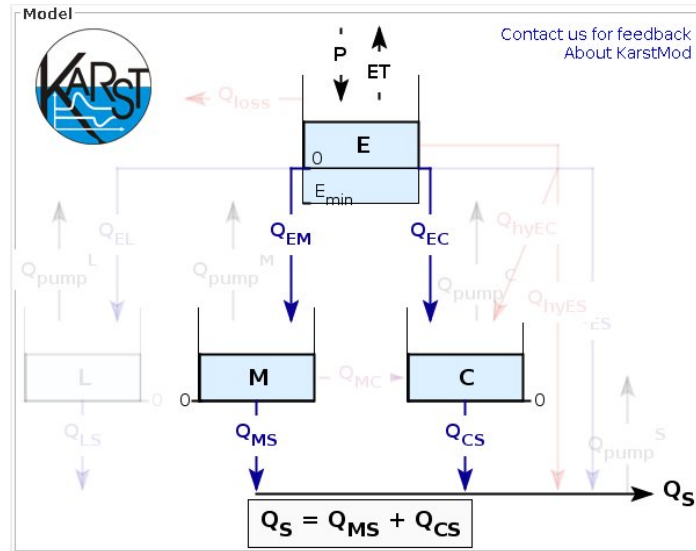


Figure 3: Model structure for the fontaine de Vaucluse hydrosystem

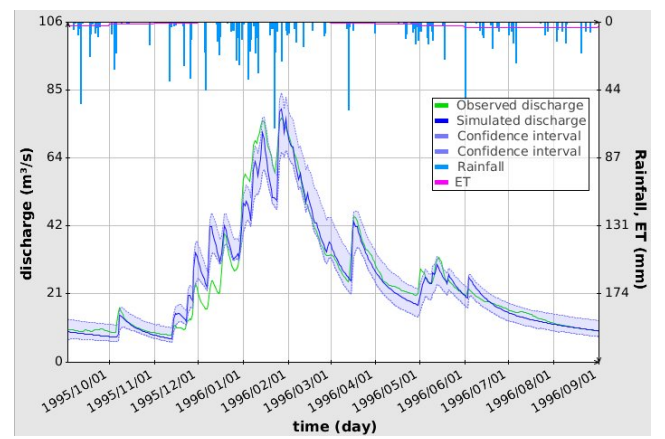
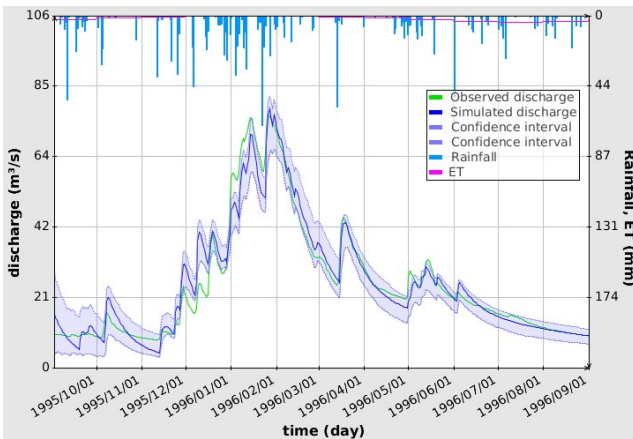


Figure 4: Simulation results for the behavioural parameter set (Nash Sutcliffe efficiency higher than 0.9) during calibration stage: (left) no warm-up period, (right) a one-year warm-up

Parameter	First-order index	Total-effect index ▼
k_{CS}	0.312	0.487
k_{EM}	0.136	0.309
k_{MS}	0.053	0.134
M_0	0.061	0.12
E_0	0.067	0.111
k_{EC}	0.011	0.088
C_0	0.051	0.083

Parameter	First-order index	Total-effect index ▼
k_{CS}	0.313	0.659
k_{EM}	0.272	0.626
k_{EC}	0.004	0.126
k_{MS}	0.001	0.024
M_0	1.094E-4	0.001
E_0	2.174E-5	7.314E-5
C_0	-2.012E-6	4.793E-8

Figure 5: Sensitivity indexes for the model: (left) no warm-up period, (right) a one-year warm-up.

3. Conclusion

The platform can be regarded as a useful tool for analyzing the hydrological processes for karst systems and for assessing the impact of management policies, for example when pumping is performed directly in the karst network. Although KarstMod has been designed for simulation of spring discharge at karst outlets, this platform could obviously be applied to any rainfall-runoff relationship modelling purpose. Thanks to its friendly interface, no programming skills are required to run the modelling platform. KarstMod will therefore prove especially useful for learning and occasional users, e.g. students. For research applications, KarstMod provides a primary analysis, easy exploration and comparison of models structures. Future developments of the platform include : (i) the consideration of the uncertainty on the measured input data in the calibration process, (ii) the proposition of additional transfer functions [10, e.g.].

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Nomenclature

$\overline{Q_{obs}}$	mean value of Q_{obs} (L^3/T)
α_{AB}	general notation for the positive exponent of the discharge-water level function from compartment A to compartment B (assumed to be positive)
α_{loss}	positive exponent for the threshold loss function (-)
ΔE_{hy}	thresholds for the deactivation of the Q_{hy} function (L)
ε_{hy}	binary indicator of the activation of the hysteretic discharge
A, B	general notation for the water level in compartment A, B (L)
E_{hy}	thresholds for the activation of the Q_{hy} function (L)
E_{loss}	threshold for the activation of the Q_{loss} function (L)
E_{min}	minimum water level in compartment E (L)
ET	evapotranspiration rate (L/T)
k_{AB}	specific discharge coefficient for linear discharge law from compartment A to compartment B (L/T)
k_{hy}	specific discharge coefficient of the hysteretic discharge (L/T)
k_{loss}	specific discharge coefficient for the Q_{loss} function (L/T)
L_{ref}	reference length for normalisation of the water level of compartment A
n_{obj}	target number of simulations to achieve $WOBJ > WOBJ_{min}$
P	precipitation rate (L/T)
p	coefficient used to define Q_{hyEC} as a function of Q_{hyES}
Q_{AB}	general notation for the discharge from compartment A to compartment B per unit surface area (L/T)
Q_{hyEC}	hysteretic discharge from compartment E to compartment C per unit surface area (L/T)
Q_{hyES}	hysteretic discharge from compartment E to the outlet S per unit surface area (L/T)
Q_{hy}	total hysteretic discharge from compartment E per unit surface area (L/T)
Q_{loss}	discharge lost from compartment E per unit surface area (L/T)
Q_{obs}	observed discharge (L^3/T)
Q_{pump}^A	discharge rates outtaken from compartment A per unit surface area (L)
Q_S	discharge at the outlet (L^3/T)
R_A	recharge area (L^2)
sgn	signum function

t_{max}	maximum simulation duration (T)
w	coefficient $\in [0, 1]$ used for weighting the performance criteria (-)
A, B	general notation for the compartments: either E, L, M, C, and the outlet: S
BE	balance error (-)
NSE	Nash-Sutcliffe efficiency model performance criteria
WOBJ	objective function
$WOBJ_{min}$	threshold value of the objective function

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