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Improvement of the KarstMod modeling platform for a better assessment of karst groundwater resources

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Abstract.

Hydrological models are fundamental tools for the characterisation and management of karst systems. We propose an updated version of KarstMod, a software dedicated to lumped parameter rainfall-discharge modeling of karst aquifers. KarstMod provides a modular, user-friendly modeling environment for educational, research and operational purposes. It also includes numerical tools for time series analysis, model evaluation and sensitivity analysis. The modularity of the platform facilitates common operations related to lumped parameter rainfall-discharge modeling, such as (i) set up and parameter estimation of a relevant model structure, and (ii) evaluation of internal consistency, parameter sensitivity and hydrograph characteristics. The updated version now includes (i) external routines to better consider the input data and their related uncertainties, i.e. evapotranspiration and solid precipitation, (ii) enlargement of multi-objective calibration possibilities, allowing more flexibility in terms of objective functions as well as observation type and (iii) additional tools for model performance evaluation including further performance criteria and tools for model errors representation.

1 Introduction

Karst systems consist of heterogeneous aquifers characterized with the co-existence of three types of porosity: (i) inter-granular porosity, (ii) fracture porosity and (iii) large voids and conduits (Palmer, 1991; White, 1999) characterized by contrasted hydrodynamic properties. The existence of surface karst features such as shafts or swallow holes often leads to concentrated point-source recharge towards karst conduits in addition to the more common homogeneous diffuse recharge over the catchment. It also implies that flow regimes can be either laminar or turbulent. Karst aquifers constitute an essential source of drinking water for about 9.2% of the world population (Stevanović, 2019) and it is estimated that one-quarter of the world population depends on freshwater from karst aquifers (Ford and Williams, 2013). Karst aquifers contain an important volume of freshwater while only 1% of its annually renewable water is used for drinking water supply (Stevanović, 2019). Karst

groundwater thus represents an unique opportunity to limit the imbalance between growing demand and limited freshwater resource (Wada et al., 2016; Bierkens and Wada, 2019), particularly in areas where no other freshwater resources are identified. However, karst aquifers are also particularly vulnerable to potential sources of contamination, including emergent contaminants (Lukač Reberski et al., 2022), residues of phyto-sanitary products (Lorette et al., 2022) and wastewater (Doummar et al.,

25 2022). Understanding the functioning of karst aquifers and developing operational tools to predict the evolution of freshwater resources is therefore a major challenge for the hydrological science community (Blöschl et al., 2019). Such tools are also required for a better assessment of groundwater vulnerability as well as sustainable management of the groundwater resources (Elshall et al., 2020).

KarstMod is an adjustable modeling platform (Mazzilli et al., 2019) dedicated to lumped parameter rainfall-discharge mod-

30 eling allowing for (i) simulation of spring discharge, piezometric head and surface discharge, (ii) hydrodynamic analysis of the internal fluxes considered in the model, (iii) model performance evaluation and parametric sensitivity analysis. In this paper, we present the new features incorporated in KarstMod: (i) external routines to better consider the input data and their related uncertainties, i.e. evapotranspiration and solid precipitation, (ii) enlargement of multi-objective calibration possibilities, allowing more flexibility in terms of objective functions as well as observation type with the possibility to include surface water

35 discharge in the calibration procedure and (iii) model performance evaluation, including additional performance criteria as well as additional tools for model errors representation such as the diagnostic efficiency plot (Schwemmle et al., 2021). Also, we present two case studies to illustrate how KarstMod is useful in the framework of the assessment of karst groundwater resources and its sensitivity to groundwater abstraction. Section 2 is devoted to the presentation of the background and motivations to improve the functionalities of the platform while Sect. 3 presents the main features of KarstMod. Section 4 illustrates the

40 application of rainfall-discharge modeling using KarstMod within the Touvre (western France) and the Lez (southern France) karst systems, which both constitute strategic fresh water resources and ensure drinking water supply.

2   Background and motivations

2.1   Challenges in karst groundwater resources

Karst aquifers are affected by the combination of different components of global change such as (i) effects of climate change

45 which are particularly pronounced in the Mediterranean area (Dubois et al., 2020; Nerantzaki and Nikolaidis, 2020), (ii) increasing groundwater abstraction (Labat et al., 2022), as well as (iii) changes in land cover land use (Bittner et al., 2018; Sarrazin et al., 2018). Therefore, the assessment of karst groundwater resources vulnerability in the present context requires operational tools for estimating the sustainable yield of karst aquifers but also to predict the impacts of climatic or anthropogenic forcing on groundwater resources in the long term (Sivelle et al., 2021). In order to address these issues, different

50 modeling approaches have been developed (Jeannin et al., 2021) such as, among others, fully-distributed models (Chen and Goldscheider, 2014), semi-distributed models (Doummar et al., 2012; Dubois et al., 2020; Ollivier et al., 2020), and lumped parameter models (Mazzilli et al., 2019) including semi-distributed recharge (Bittner et al., 2018; Sivelle et al., 2022a). Among these, lumped parameter models are recognized as major tools to explore the ability of conceptual representations to explain

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observations in karst systems (Poulain et al., 2018; Sivelle et al., 2019; Duran et al., 2020; Frank et al., 2021) and for managing
55   karst groundwater resources (Sivelle and Jourde, 2020; Sivelle et al., 2021; Labat et al., 2022; Cousquer and Jourde, 2022).

2.2   Challenges in lumped parameters modeling in karst hydrology

Lumped parameter models consist of a functional approach that analyzes an hydrogeological system at the catchment scale
and describes the transformation from rainfall into discharge using empirical or conceptual relationships. Therefore, parameter
values or distributions cannot be determined directly from catchment physical characteristics or *in-situ* measurements, excepted
60   the discharge coefficient to the spring that can be estimated on the basis of recession curve analysis. Instead, model parameters
values must be estimated by history-matching. In a general way, rainfall-discharge models in karst hydrology are calibrated
considering spring discharge measurements.

Former studies have shown the interest of considering various type of observations such as natural hydro-chemical tracers:
NO_3 and SO_4 concentrations (Hartmann et al., 2013), electrical conductivity (Chang et al., 2021) or excess air (Sivelle et al.,
65   2022b). Indeed, the consideration of complementary observation data in groundwater model calibration appears relevant in
many applications (Schilling et al., 2019) but requires additional investigations before a suitable implementation in Karst-
Mod. Therefore, in this paper, we will focus on the use of hydrodynamics observations only. Indeed, considering piezometric
head variations in lumped parameters rainfall-discharge models may lead to better model performance (Mazzilli et al., 2011;
Cousquer and Jourde, 2022). Nonetheless, the information content of the piezometric head time series (directly measured, or
70   derived from ground-based gravity measurements) for lumped parameters rainfall-discharge models calibration purpose can
be disputable when the available data is not adequate to characterize the whole catchment due to the important heterogeneity
in karst aquifers (Sivelle and Jourde, 2020; Mazzilli et al., 2013). Also, Cousquer and Jourde (2022) account for the surface
runoff in a lumped parameters rainfall-discharge model calibration procedure allowing to reduce the parametric uncertainties.

Another key point in lumped parameter rainfall-discharge modeling concerns the evaluation of the meteorological forcing,
75   i.e. precipitation (P) and evapotranspiration (ET). The transformation of precipitation into recharge and finally into discharge
includes several processes with characteristic times covering several orders of magnitude (Blöschl and Sivapalan, 1995). Thus,
the temporal resolution of the hydrological model must be suitable in the range of time and space scale where the physical
phenomenons take place. Coupling hydrological models at multiple temporal resolutions can provide a better model consis-
tency (Sivelle et al., 2019) since the transfer function in karst aquifers may present short response time. Also, errors in rainfall
80   time series can significantly affect model parameters and structure (Oudin et al., 2006). Finally, the response of karst spring
discharge is sensitive to energy and water fluxes within the soil-vegetation-atmosphere (SVA) continuum as well as changes
in climatic conditions (Hartmann et al., 2017). Bittner et al. (2021) computed several models to evaluate the fluxes related to
interception, evapotranspiration and snow process. The results show significant uncertainties related to input data as well as
potential compensation between the various uncertain processes. In some cases, snow melt is a controlling factor in the water
85   balance (Doummar et al., 2018a; Liu et al., 2021), thus a suitable snow melt estimation is required to improve hydrological
model performance (Çallı et al., 2022). Therefore, two meteorological modules have been added to KarstMod: (i) a "Snow

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routine" and (ii) a routine to compute the potential evapotranspiration (PET), denoted "PET routine". The two additional modules allow to better account for snow and evapotranspiration processes.

3 Implementation

90 The updated version of KarstMod implements additional features to enhance the rainfall-discharge modeling practices. First, we describe the additional modules (snow and PET routines) for a better meteorological forcing estimation. Then, we introduce the additional tools proposed for (i) the set up and calibration of the model structure, (ii) model performance evaluation as well as (iii) uncertainties consideration. Figure 1 shows a screenshot of the KarstMod software.
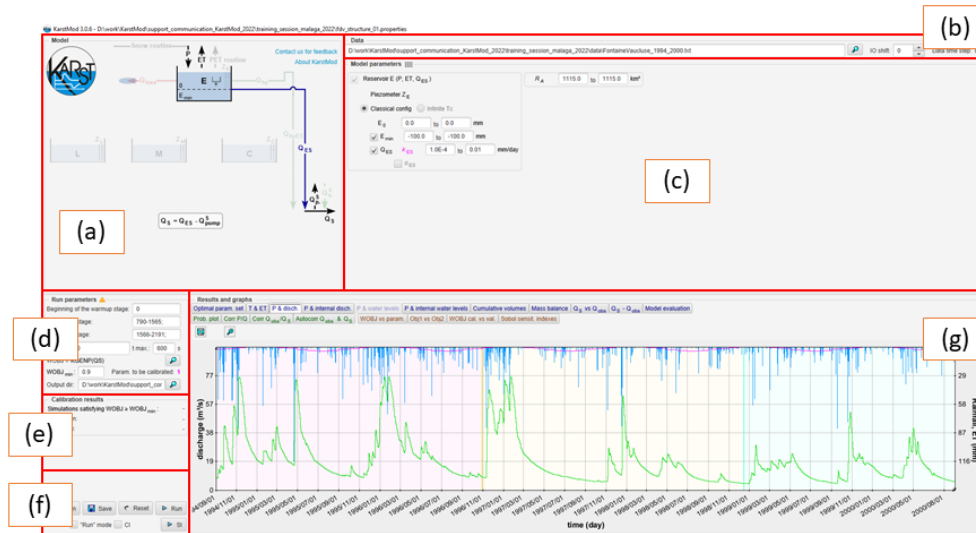

Figure 1. Screenshot of the KarstMod software with: (a) model structure, (b) data import, (c) model parameters, (d) run parameters, (e) calibration results, (f) command bar and (g) results and graphs.

3.1 Meteorological modules

95 ### 3.1.1 Snow routine

KarstMod allows using either observation-based precipitation time series P [L T^{-1}] or estimated precipitation time series Psr [L T^{-1}] using a snow routine. The latter is similar to the one used by Chen et al. (2018) – without the radiation components – which has been successfully used for improving the simulation of karst spring discharge in snow-covered karst systems (Chen et al., 2018; Cinkus et al., 2023b). It consists of a modified HBV-snow routine (Bergström, 1992) for simulating snow

100 accumulation and melt over different sub-catchments based on altitude ranges (appendix A). The estimated precipitation Psr gives the water leaving the snow routine, equivalent to the recharge into the first compartment of the model (compartment E in KarstMod). Psr^* for each sub-catchment is proportional to its surface regarding the complete catchment area. The snow

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routine workflow requires both air temperature T [°C] and precipitation P [L T^{-1}] time series. P is considered as snow when T in the sub-catchment is lower than the temperature threshold T_s. Snow melt starts when the temperature exceeds the threshold according to a degree-day expression. The snow melt is a function of the melt coefficient MF [L T^{-1} °C^{-1}], and the degrees above the temperature threshold T_s. Runoff starts when the liquid water holding capacity of snow CWH [-] is exceeded. The refreezing coefficient CFR [-] stands for refreezing liquid water in the snow when snow melt is interrupted (Bergström, 1992). The output of the snow routine consists of a redistributed precipitation time series Psr. The four parameters of the snow routine (i.e. T_s, MF, CWH and CFR) can be considered in the parameter estimation procedure as well as sensitivity analysis. The snow routine features can be activated from the model structure area (Figure 1a).

3.1.2 PET routine

An additional module allows to compute PET based on the Oudin's formula (Oudin et al., 2005). The PET routine can be activated from the model structure area (Figure 1a). Then, KarstMod allows to consider water transfer between in the soil-atmosphere continuum in four different ways (Figure 2):

(a) Effective precipitation time series ($Peff$) can be pre-processed by user (Eq. 1) and the evapotranspiration flux is not activated in the model structure selection window in KarstMod (1a).

$$Peff = P - ETa \qquad (1)$$

where $Peff$ is effective precipitation [L T^{-1}], P is precipitation [L T^{-1}] and ETa is user-defined actual evapotranspiration [L T^{-1}] computed by observation-based data or external model.

(b) User defined PET can be given as input in KarstMod for the evapotranspiration time series. Compartment E stands for a soil and epikarst storage zone, where water is available for actual evapotranspiration (ETa), flows to lower level of the model structure or outflow as surface discharge losses. Using E_{min}, user can simulate water holding capacity and non-linear behavior of karst recharge.

(c) User-defined actual evapotranspiration (ETa) can be given as input data in KarstMod for evapotranspiration time series instead of potential evapotranspiration. KarstMod computes effective precipitation by limiting the evapotranspiration to water content available in compartment E; calculated actual evapotranspiration can then be lower than user's input ETa.

(d) The new feature in KarstMod is the PET routine which estimates the potential evapotranspiration based on the Oudin's formula (Oudin et al., 2005) (Eq. 2). It needs a temperature time series and two parameters to be estimated, which can be considered in the parameter estimation procedure as well as sensitivity analysis.

$$PET = \frac{R_e}{\lambda.\rho} \times \frac{T + K2}{K1} \quad if \quad T + K2 > 0 \quad else \quad PET = 0 \qquad (2)$$

where R_e is the extraterrestrial radiation [MJ L^{-2} T^{-1}] depending only on latitude Lat and Julian day, λ is the latent heat flux (taken equal to 2.45 MJ M^{-1}), ρ is the density of water [M L^{-3}] and T is the mean daily air temperature [°C]. The

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latter is a single function of the Julian day for a given location. $K1$ [°C] and $K2$ [°C] are constants to adjust over the catchment for rainfall-discharge model (Oudin et al., 2005). In KarstMod, both $K1$ and $K2$ can be considered in the parameter estimation procedure as well as sensitivity analysis.
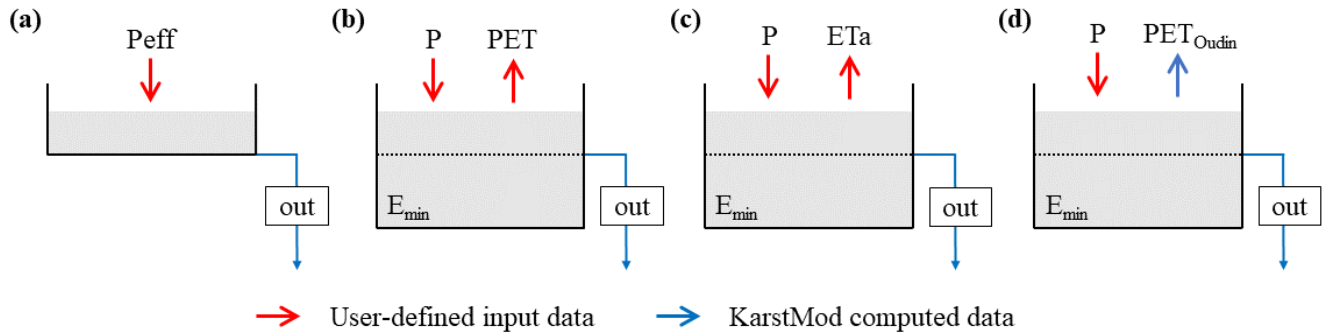

Figure 2. The four ways to account for evapotranspiration in KarstMod. The user can provides either (a) a self computed effective precipitation (P - ETa) as a single input time series, (b) both P and PET time series, (c) both P and ETa and (d) both P and T time series. P is precipitation, ETa is actual evapotranspiration, PET is potential evapotranspiration and PET_{Oudin} is KarstMod's computed potential evapotranspiration with Oudin's formula.

3.2   Set up and calibration of the model structure

The modular structure proposed in KarstMod is based on a widely used conceptual model which separates karst aquifers into an infiltration zone and a saturated zone, or low and quick flows through the unsaturated and saturated zones (Fleury et al., 2007, 2009; Guinot et al., 2015; Mazzilli et al., 2019; Sivelle et al., 2019). Based on this conceptual representation, the platform offers four compartments organized as a two-level structure: (i) compartment E (higher level) and (ii) compartments L, M and C (lower level). A priori, the higher-level stands for the infiltration zone or the soil and epikarst. At the lower level, compartments L, M, and C stand for the different sub-systems of the saturated zone, or for low and quick flows of the whole hydrosystem. The various model structures and their governing equations are presented in Mazzilli et al. (2019, 2022). Also, KarstMod allows to perform hydrological modeling on both daily and hourly temporal resolutions (Sivelle et al., 2019).

The user can activate (or deactivate) the various compartments (E, L, M and C) within the "model structure" panel (Figure 1a). The solid and faded colors represent the activated and the inactivated features respectively. The fluxes and their activation thresholds as well as the exponent of the discharge law α (in case of non-linear discharge law such $\alpha \neq 1$) are managed from the "model parameters" panel (Figure 1c). The user can account for pumping Q_{pump} (water coming out of the compartment) as well as sinking stream Q_{sink} (water coming into the compartment). Such option is available only if the user provides the required time series (Figure 1b).

The user must provide the warm-up, calibration and validation periods (Figure 1d). The warm-up period must be set in order to be independent from initial conditions to avoid bias in the parameter estimation procedure (Mazzilli et al., 2012). Then, a

calibration period (i.e. the period in which the parameter are estimated to reduce the predictive errors) and a validation period (i.e. period separated from the calibration period) can be defined to run the split sample test procedure (Klemeš, 1986). For calibration purpose, KarstMod proposes several widely used performance criteria ϕ: the Pearson's correlation coefficient r_p (Freedman et al., 2007), the Spearman rank correlation coefficient r_s (Freedman et al., 2007), the Nash-Sutcliffe Efficiency NSE (Nash and Sutcliffe, 1970), the volumetric error VE (Criss and Winston, 2008), the modified balance error BE (Perrin et al., 2001), the Kling-Gupta Efficiency KGE (Gupta et al., 2009) and a non-parametric variant of the Kling-Gupta Efficiency $KGENP$ (Pool et al., 2018). To compute a multi-objective calibration procedure the user can create his own objective function Φ as a weighted sum of several objective functions:

$$\Phi = \sum_{i=1}^{N} \omega_i \times \phi_i(U) \tag{3}$$

where ω is the weight affected to the objective function $\phi(U)$ with $\sum w_i = 1$ and U a general notation for the observations used for parameter estimation purpose. In the KarstMod modeling platform U corresponds to either spring discharge Q_s, piezometric head measurements Z (available for compartments E, L, M and C) or surface water discharge Q_{loss} from compartment E. Also, the objective function ϕ can be computed on transformed U to avoid high water level bias on quadratic error. The following transformation are available in KarstMod: $1/U$, $\sqrt{U}$, $1/\sqrt{U}$. Therefore, the user can use any combination of the objective function ϕ, observations U and variable transformations. Depending on the modeling purpose, the user must refer to the literature to define the suitable objective function (Bennett et al., 2013; Ferreira et al., 2020; Hauduc et al., 2015; Jackson et al., 2019).

The model is calibrated using a quasi Monte-Carlo sampling procedure with a Sobol sequence sampling of the parameter space (Sobol, 1976). The procedure consists in finding an ensemble of parameter set providing an objective function Φ greater than the user defined value. The calibration procedure is stopped when either the user-defined maximum duration t_{max} is reached or the user-defined number of parameter set n_{max} are collected. KarstMod offers a "run" option allowing to run the model for user-defined parameter set, without calibration procedure, and so allowing to investigate "by-hand" the parameter space and the sensitivity of the model to specific parameters.

3.3 Model evaluation

The model performance can be evaluated for both the calibration and validation periods. It allows (i) to ensure the robustness of model predictions, even under changing conditions (which is a key point for the assessment of climate change impact) and (ii) to avoid model over-fitting within a specific range of hydro-climatic conditions observed during the calibration period. KarstMod allows the computation of the above mentioned performance criteria for both calibration and validation periods. Even though the notation "validation" is disputable such procedure is required to evaluate both explanatory and predictive dimensions of the model structure (Andréassian, 2023). Then, KarstMod offers an ensemble of numerical tools devoted to (i) check the model consistency, i.e. explanatory dimension of the model (Beven, 2001; Shmueli, 2010), (ii) evaluate the model performance, i.e. predictive dimension of the model structure.

To check the model consistency, the simulation based on the parameter set that provides the highest objective function value can be analyzed through an ensemble of graphs such as (i) internal and external fluxes as a function of time, (ii) cumulative volumes for both observed and simulated time series for spring discharge Q_s and surface water discharge Q_{loss}, (iii) simulated mass-balance as function of time, (iv) comparison of observations and simulations for either Q_s or Q_{loss} with probability function plots, auto-correlogram of the spring discharge time series, cross-correlogram of precipitation-discharge time series.

To evaluate the model performance, KarstMod offers a "Model evaluation" panel available from the graphs panel (Figure 1g) that includes several sub-panels, from the left to the right:

- The diagnostic efficiency DE (Schwemmle et al., 2021) which consists of a diagnostic polar plot that facilitates the model evaluation process as well as the comparison of multiple simulations. The DE accounts for constant, dynamics and timing errors, and their relative contribution to the model errors. Also, the decomposition of the errors between the periods of high flows and low flows allows to better investigate the model bias, as well as to provide critical evaluation for impact studies, particularly for the assessment of climate change impacts. Indeed, the accurate evaluation of low flow periods (in terms of frequency, intensity and duration) becomes more and more crucial for groundwater resource variability assessment.

- The available objective functions ϕ are presented as a radar chart which consists of a polygon where the position of each point from the center gives the value of the performance criteria. The closer the point is to the outside of the radar chart, the better the model performs. The radar chart is made for both calibration and validation periods and for each of the calibration variables considered in the modeling (Q_s, Z_{obs}^A with A for either E, M, C or L compartments and Q_{loss}).

- The KGE (Gupta et al., 2009) consists of a diagonal decomposition of the NSE (Nash and Sutcliffe, 1970) to separate Pearson's correlation coefficient r_p, representation of bias β_{KGE}, and variability α_{KGE}. Thus, the KGE is comparable to multi-objective criteria for calibration purpose (Pechlivanidis et al., 2013). The sub-panel offers (i) a bi-plot of the three KGE's components and (ii) a radar plot visualization of the KGE's components, allowing to identify potential counterbalancing errors according to these different components (Cinkus et al., 2023a). The two above mentioned plots also include the decomposition of the $KGENP$ (Pool et al., 2018) in terms of Spearman's rank correlation coefficient r_s, representation of bias β_{KGENP} and non-parametric variability α_{KGENP}.

3.4 Dealing with uncertainties

Moges et al. (2021) summarize the various source of uncertainties in hydrological models including structural and parametric uncertainties as well as uncertainties related to input data and observations. The latter concern both the input (i.e. precipitation and evapotranspiration) and the output (i.e. discharge) of the modeled systems. Many references are devoted to the uncertainties related to input data and observations. As an example, Westerberg et al. (2020) include information about the discharge uncertainty distribution in the objective function and perform better discharge simulation. Also, the precipitation error can be dependent on the data time step (McMillan et al., 2011) and could impact the hydrological model performance (Ficchì et al., 2015). Lumped parameter hydrological models generally consider meteorological time series representative of a whole

catchment, which may require some pre-processing, particularly for snow processes since it can have a strong influence on flow dynamics. Thus, KarstMod includes variables related to both the snow routine (i.e. the redistributed precipitation time series Psr) and the PET routine (i.e. estimated potential evapotranspiration PET) in the parameter estimation procedure. This allows to investigate the sensitivity of the flow simulation to these input data, when using snow and PET routines. Nonetheless, KarstMod does not include features to investigate the impact of observation uncertainties on the parameter estimation.

As many environmental problems, parameter estimation in rainfall-discharge modeling consists generally in ill-posed problems, i.e. the modeling encounters issues about the unicity, identifiability and stability of the problem solution (Ebel and Loague, 2006). As a consequence, several representations of the modeled catchment may be considered as equally acceptable (Beven, 2006). Knoben et al. (2020) evaluate the performance of 36 daily lumped parameter models over 559 catchments and show that between 1 and up to 28 models can show performance close to the model structure with the highest performance criteria. Such results are widely covered in catchment hydrology (Zhou et al., 2021; Pandi et al., 2021; Dakhlaoui and Djebbi, 2021; Darbandsari and Coulibaly, 2020; Gupta and Govindaraju, 2019) but still poorly investigated in karst hydrology. Indeed, the structural uncertainty impacts on rainfall-discharge modeling in karst hydrology is not properly evaluated whereas many studies consider several hydrological model structure to include structural uncertainty in flow simulation (Hartmann et al., 2012; Jiang et al., 2007; Jones et al., 2006; Sivelle et al., 2021). KarstMod includes more than 50 combinations of the various compartments as well as various compartments model (i.e. compartment with linear or non-linear discharge law and compartment with infinite characteristic time) and allows a quick implementation of the various model structures. The user can easily manage to start the modeling with one single compartment and gradually move to more complex model structure with up to 4 compartments, 5 fluxes connected to the spring, 4 internal fluxes and 1 flux running out of the system.

Considering each model structure, parametric equifinality can be investigated using (i) dotty plots of the values of the objective function against the parameter values, (ii) dotty plot of the values of the performance criteria used to define the aggregated objective function, and (iii) the variance-based, first-order S_i and total S_{Ti} sensitivity indexes for the model parameters. Details concerning the computation of sensitivity indexes within KarstMod are given in Mazzilli et al. (2019, 2022).

4 Examples of application

To illustrate KarstMod application and the use of the above presented functionalities for the assessment of karst groundwater resources, we propose two case studies: (i) the Touvre karst system and (ii) the Lez karst system. Both karst systems consist of strategic freshwater resources for drinking water supply (DWS), for the city of Angoulême (western France) and Montpellier (southern France) respectively.

4.1 The Touvre karst system (La Rochefoucauld)

The Touvre karst system is a karst system where the infiltration consists of (i) a delayed infiltration of effective rainfall on karstic recharge area and (ii) a direct infiltration of surface water from the Tardoire, Bandiat, and Bonnieure rivers. The latter are surface stream flows within metamorphic rocks that partly infiltrate to subterranean at the contact with sedimentary formations,

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mainly composed of Middle to Upper Jurasic limestones. The springs of the Touvre, located 7 km east of Angoulême (western France), have three main outlets (the Bouillant, the Dormant and the Font de Lussac) and a secondary outlet (the Lèche) (Labat et al., 2022). In the following, the discharge of the four outlets are accumulated and named Touvre spring.

The Touvre karst system constitutes a strategic freshwater resource for drinking water supply (DWS) of Angoulême, with around 110,000 inhabitants, but also contributes to water supply for industry and agriculture. In 2015, there were 84 pumping wells over the karstic impluvium of the Touvre karst system, and around 100 more in the Tardoire, Bandiat, and Bonnieure rivers catchment. Based on the data provided by the Adour-Garonne Water Agency, the annual groundwater abstraction for agriculture represents 4.6 Mm^3 whereas annual groundwater abstraction for DWS represents 1.1 Mm^3 over the karstic impluvium of the Touvre karst system. On the three rivers catchment (out of the karstic impluvium), the annual groundwater abstraction represents 2.5 Mm^3 for agriculture and 3.3 Mm^3 for DWS, mainly through river intakes or alluvial groundwater abstraction. The total annual volume of abstracted groundwater in the area represents around 5 % of the annual volume of transit at the Touvre spring. This is quite low compared with karst aquifers in France exploited for their groundwater resource, such as the Lez spring (Jourde et al., 2014) and the Oeillal's spring karst catchment (Sivelle et al., 2021), where the annual groundwater abstraction volume represents respectively 50 % and 15 % of annual volume of transit at the spring. Therefore, the Touvre karst system seems not to be over exploited at the moment but the impact of groundwater abstraction should be addressed in the context of global change to ensure a sustainable management of this strategic fresh water resource.

The area is characterized by an ocean influenced climate with a mean annual precipitation around 800 mm/year distributed over an average of 255 rainy days. The estimation is performed with Thiessen polygon methods based on eleven meteorological stations over the area (Labat et al., 2022). The mean annual potential evapotranspiration is around 770 mm/year according to the Penman-Monteith estimation provided by the French meteorological survey (Météo-France). The Touvre daily spring discharge shows a significant variability ranging from 3 m^3/s to 49 m^3/s with a coefficient of variation around 0.46 (Figure 4b). The surface stream flow rates for the Bonnieure, Bandiat and Tardoire rivers are concentrated within the autumn and winter periods. During the summer period, the discharge in the three rivers are very low (Figure 4c). The more significant groundwater abstraction is performed during the summer period, while the Touvre spring discharge reaches its lowest values within the late summer and early autumn periods (Figure 4, c and d).

Figure 3 shows the model structure for the Touvre karst system that consists of three compartments organized in two levels (Labat et al., 2022). The upper level corresponds to reservoir E and represents both the unsaturated part of the system and a temporary aquifer. This reservoir is connected with the two reservoirs of the lower level: C (Conduit) and M (Matrix) representative of quick and slow flow dynamics respectively. The upper level of the model structure is affected by precipitation P and potential evapotranspiration PET while the lower level of the model structure is affected by (i) groundwater abstraction and (ii) sinking river stream-flow from the surface to underground. Figure 4 shows the various time series required for the hydrological modeling of the Touvre karst system. The methodology for daily time series preparation given in Labat et al. (2022) allows to account for the influence of groundwater abstraction on transmissive or capacitive part of the karst aquifer as well as the influence of concentrated and diffuse infiltration of the surface river stream-flow.
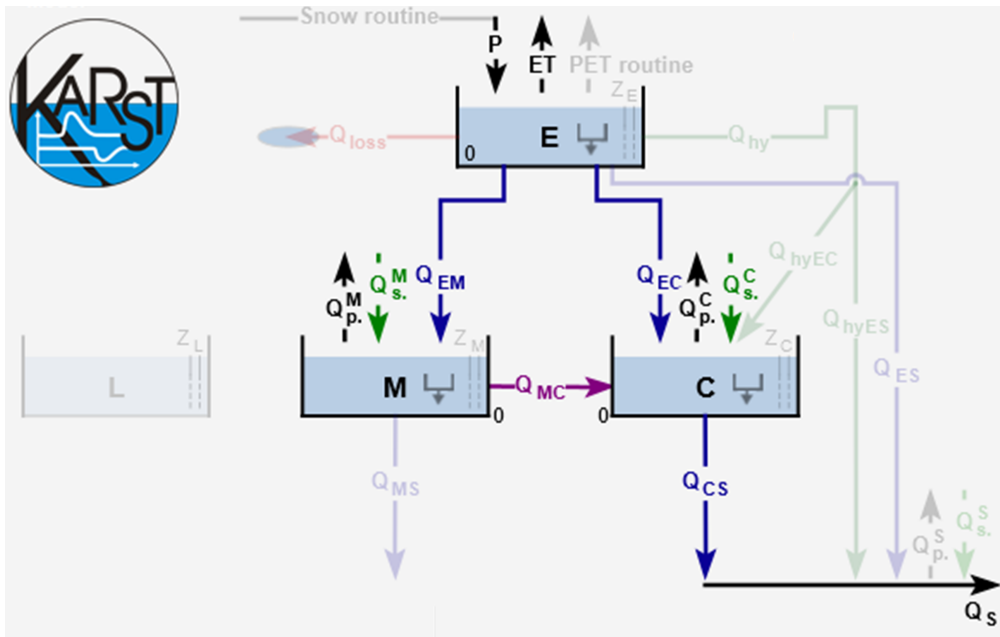
Figure 3. Screenshot of KarstMod with a focus on the panel "Model structure" for the Touvre karst system. The solid lines correspond to the activated fluxes whereas the faded color lines are not activated. $Q_{p.}^M$ and $Q_{p.}^C$ stand for groundwater abstraction that affects compartments M and C respectively while $Q_{s.}^M$ and $Q_{s.}^C$ stand for sinking flow that affects compartments M and C respectively.
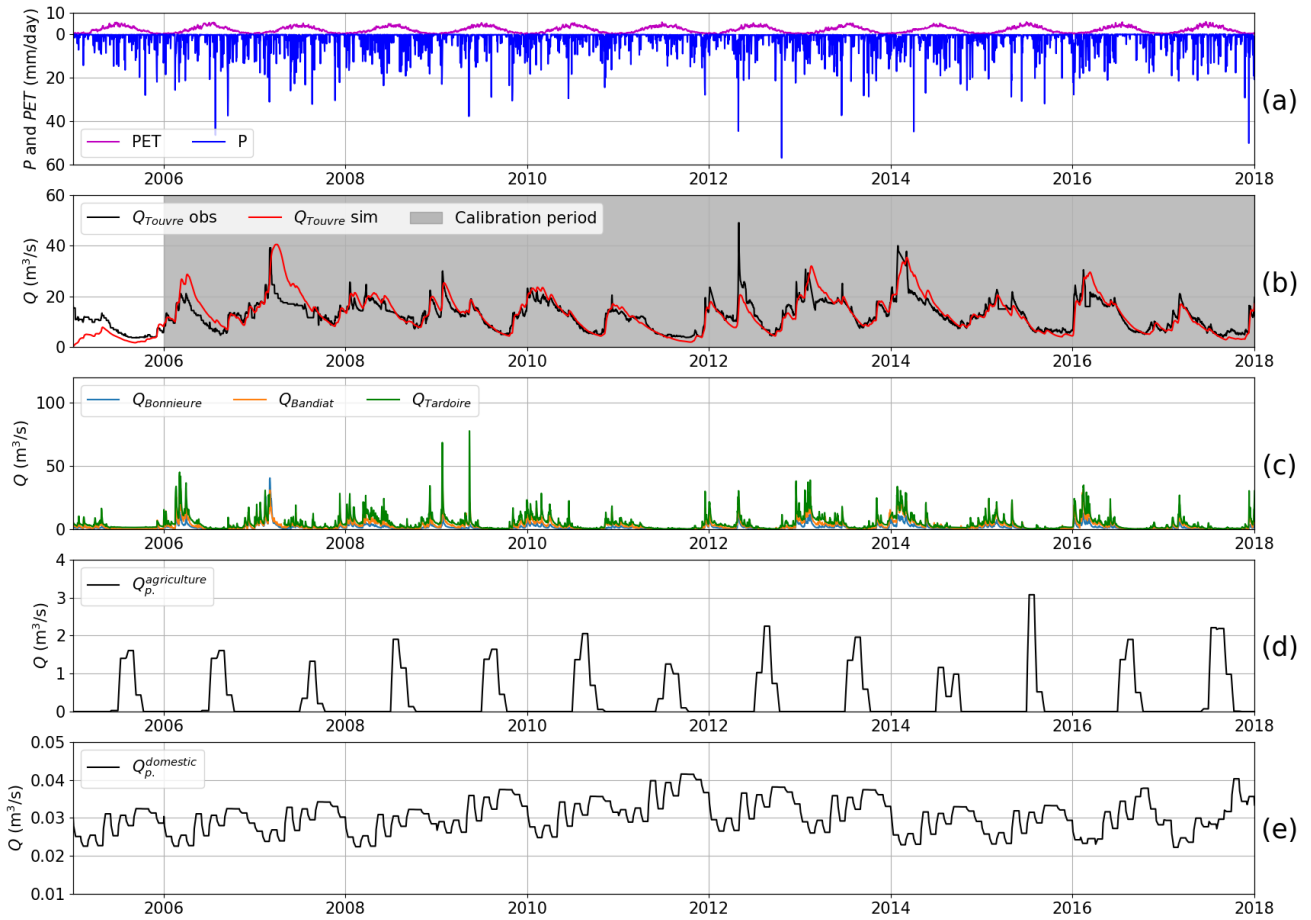
Figure 4. Daily time series for the Touvre system: a) precipitation (P) and potential evapotranspiration (PET), b) observed and simulated karst spring discharge (Q_{Touvre} obs and Q_{Touvre} sim), c) observed river streamflow discharge ($Q_{Bonnieure}$, $Q_{Bandiat}$, $Q_{Tardoire}$), d) and e) groundwater abstraction discharge ($Q_{p.}^{agriculture}$, $Q_{p.}^{domestic}$).

The objective of the hydrological modeling is to assess the impact of groundwater abstraction on spring discharge, and more particularly during low flow periods (Labat et al., 2022). So, the calibration is performed according to the $KGENP$ that improve the simulations during mean and low-flow conditions using the Spearman rank correlation due to it insensitivity to extreme values (Pool et al., 2018). The sampling procedure is set up to find $n_{obj} = 5000$ simulations with $KGENP$ greater than 0.9. Afterwards the model is evaluated using the various features proposed in KarstMod (Figure 5). The diagnostic efficiency plot (Figure 5a) testifies of several elements: (i) the model seems to slightly overestimate high flow and underestimate low flow, (ii) the timing error is about 0.9, testifying of suitable flow dynamics in the model, (iii) low flow periods contribute more to the model errors, and (iv) there is no offset in the simulated spring hydrograph. The radar chart (Figure 5b) shows a good equilibrium between the various objective functions which values are greater than 0.8, excepted for the NSE criteria (NSE

= 0.75). It is the consequence of the design of this criteria that tends to overweight the errors during floods. Here the NSE value still greater than 0.7 and testifies of a "very good" fit according to Moriasi et al. (2007). Finally, the decomposition of the KGE (Figure 5 c and d) shows r_p = 0.91, α = 1.15 and β = 1.02 testifying of accurate dynamics and low bias, but slightly too high variability.
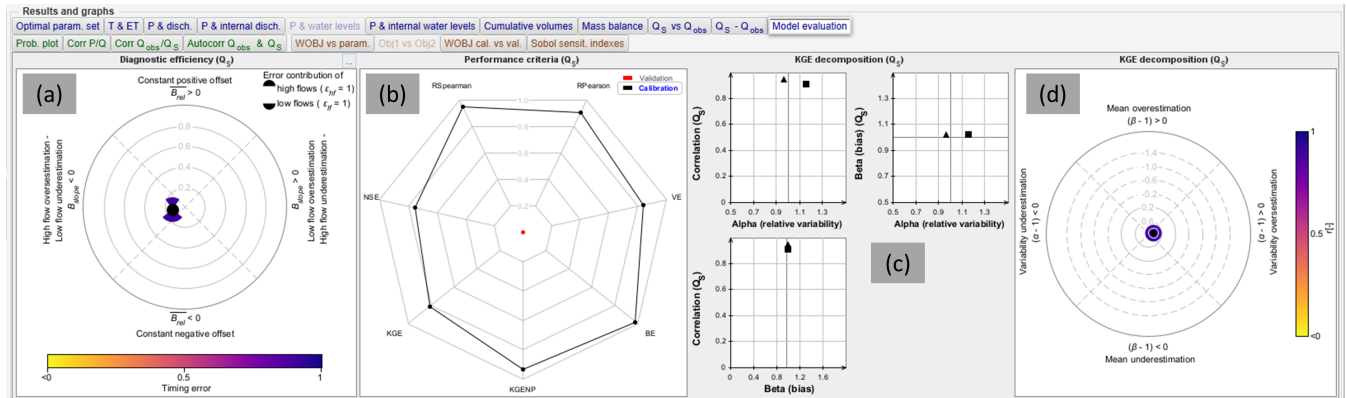

Figure 5. Screenshot of KarstMod with a focus on the sub-panel "Model evaluation". Application for the model evaluation on the Touvre system: (a) diagnostic efficiency plot (Schwemmle et al., 2021), (b) radar chart of the objective functions, (c) bi-plot of the KGE's (square) and $KGENP$'s (triangle) components, and (d) radar chart of the KGE's components.

4.2 The Lez spring

The Lez spring (southern France) consists of the main outlet of a karst system encompassed in the North Montpellieran Garrigue hydrogeological unit delimited to the west by the Herault river, and to the north and east by the Vidourle river. The geology in the area corresponds to the Upper Jurassic layers separated by the Corconne-Matelle fault (oriented N30°), leading to two main compartments in the aquifer (Bérard, 1983; Clauzon et al., 2020). The karst aquifer is unconfined in the western compartment and is locally confined in the eastern compartment. The Lez spring is located about 15 km north of Montpellier. It is of Vauclusian-type with an overflow level at 65 m a.s.l, and a maximum daily discharge of approximately 15 m^3 s^{-1}. The area is characterized by a typical Mediterranean climate with dry summers and rainy autumns. Over the 2009-2019 period, the mean annual precipitation is around 900 mm/year distributed over an average of 133 rainy days (estimation with Thiessen polygon methods based on four meteorological stations over the area: Prades-le-Lez, Saint-Martin-de-Londres, Sauteyrargues and Valflaunès), a mean annual potential evapotranspiration is around 900 mm/year according to the estimation based on Oudin's formula with the temperature measured at Prades le Lez station while the mean annual evapotranspiration is around 450 mm/year (eddy covariance flux-station of Puéchabon).

Since 1854, the Lez spring supplies the drinking water to Montpellier city and the surroundings. It currently constitutes the main fresh water resource for around 350,000 people in the area. The present water management scheme allows pumping at higher rates than the natural spring discharge during low flow periods, while supplying a minimum discharge rate ($\backsim$ 230 l/s) into the Lez river to ensure ecological flow downstream, and reducing flood hazards via rainfall storage in autumn (Avias, 1995;

Jourde et al., 2014). The pumping plant was built in 1982 with four deep wells drilled to intercept the karst conduit feeding the
315 spring, 48 m below the overflow level of the spring. Pumping in these wells allows up to 1800 l/s to be withdrawn under low
flow periods (with an authorized maximum drawdown of 30 m), while the average annual pumping flow rate is about 1010 l/s
(over the 2008-2019 period). Due to the pumping management of the aquifer, which supplies about 30 to 35 Mm^3 of water per
year to the metropolitan area of Montpellier, the discharge at the Lez spring is often low or nil.

In the present context of global change, Mediterranean karst systems already show significant decrease in spring discharge
320 (Hartmann et al., 2012; Fiorillo et al., 2012; Smiatek et al., 2013; Doummar et al., 2018b; Nerantzaki and Nikolaidis, 2020;
Dubois et al., 2020) which could be aggravated with groundwater abstraction (Sivelle et al., 2021). The Lez spring is strongly
exposed to global change impact: (i) the Mediterranean area is identified as a climate change hot-spot (Diffenbaugh and Giorgi,
2012) where the projected warming spans 1.8–8.4°C according to CMIP6 and 1.2–6.6°C according to CMIP5 during the
summer period (Cos et al., 2022), and (ii) the water management scheme will have to adapt to the future need in drinking water
325 for the growing population in the area as well as changes in the fresh water consumption practice (e.g. water use restriction
order). Therefore, a sustainable water management plan for the Lez spring requires a good appreciation of the hydrological
functioning as well as operational hydrological model to properly address impacts studies. In this framework, KarstMod allows
choosing and calibrating a suitable model structure. This constitutes a first step for global change impact study that requires
prediction tools to simulate the aquifer response to various external forcing.

330 Figure 6 shows the model structure for the Lez karst catchment (Mazzilli et al., 2011) that consists of three compartments
organized in two levels. The upper level corresponds to compartment E and represents the unsaturated part of the system,
including a soil water holding capacity E_{min} and a discharge lost from the compartment Q_{loss}. The compartment E is exposed
to precipitation P and evapotranspiration ET and discharge towards the lower level of the model structure starts when the
water level exceeds the water holding E_{min}. The lower level consists of two inter-connected compartments M and C allowing
335 to reproduce the lateral exchanges, denoted Q_{MC}, between transmissive function (compartment C) and capacitive function
(compartment M) of the karst aquifer. Both M and C compartments are considered bottomless, allowing to reproduce period
of non-overflow at the Lez spring when the mean water level in the aquifer stands below 65 m a.s.l., mainly during summer
periods due to pumping in the karst conduit. Figures 7a and 7b show the various daily time series required for the hydrological
modeling of the Lez karst system (i.e. P, ET and Q_{pump}).
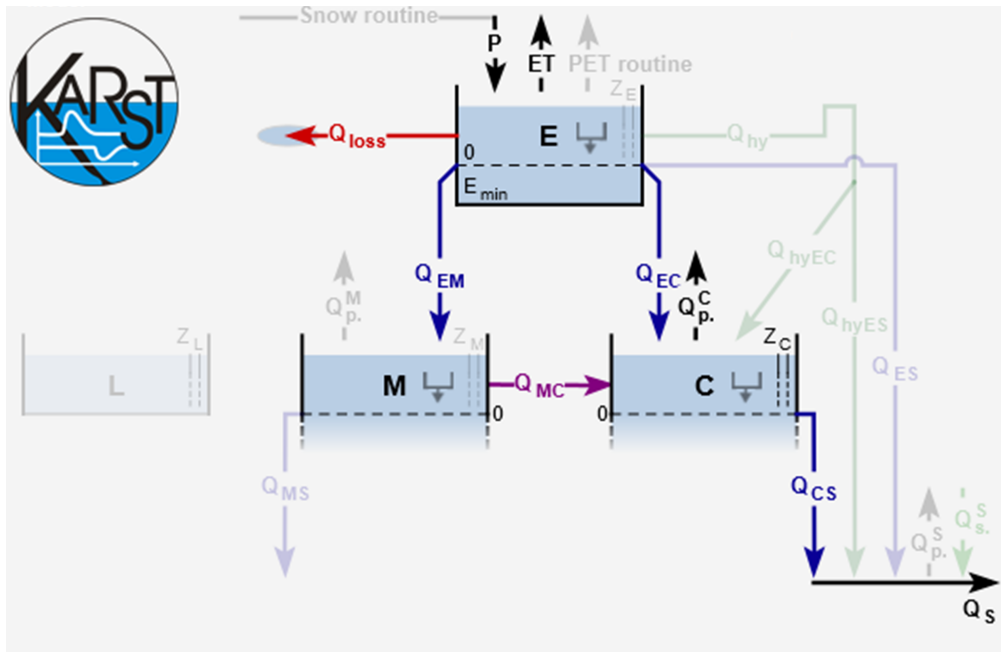
Figure 6. Screenshot of KarstMod with a focus on the panel "Model structure" for the Lez karst system. The solid lines correspond to the activated fluxes whereas the faded color lines are not activated. Q_{loss} stands for the surface discharge from the epikarst compartment, $Q_{p.}^C$ stands for groundwater abstraction that affects compartments C while Z_C stands for piezometric head measurements considered as representative of the compartment C.
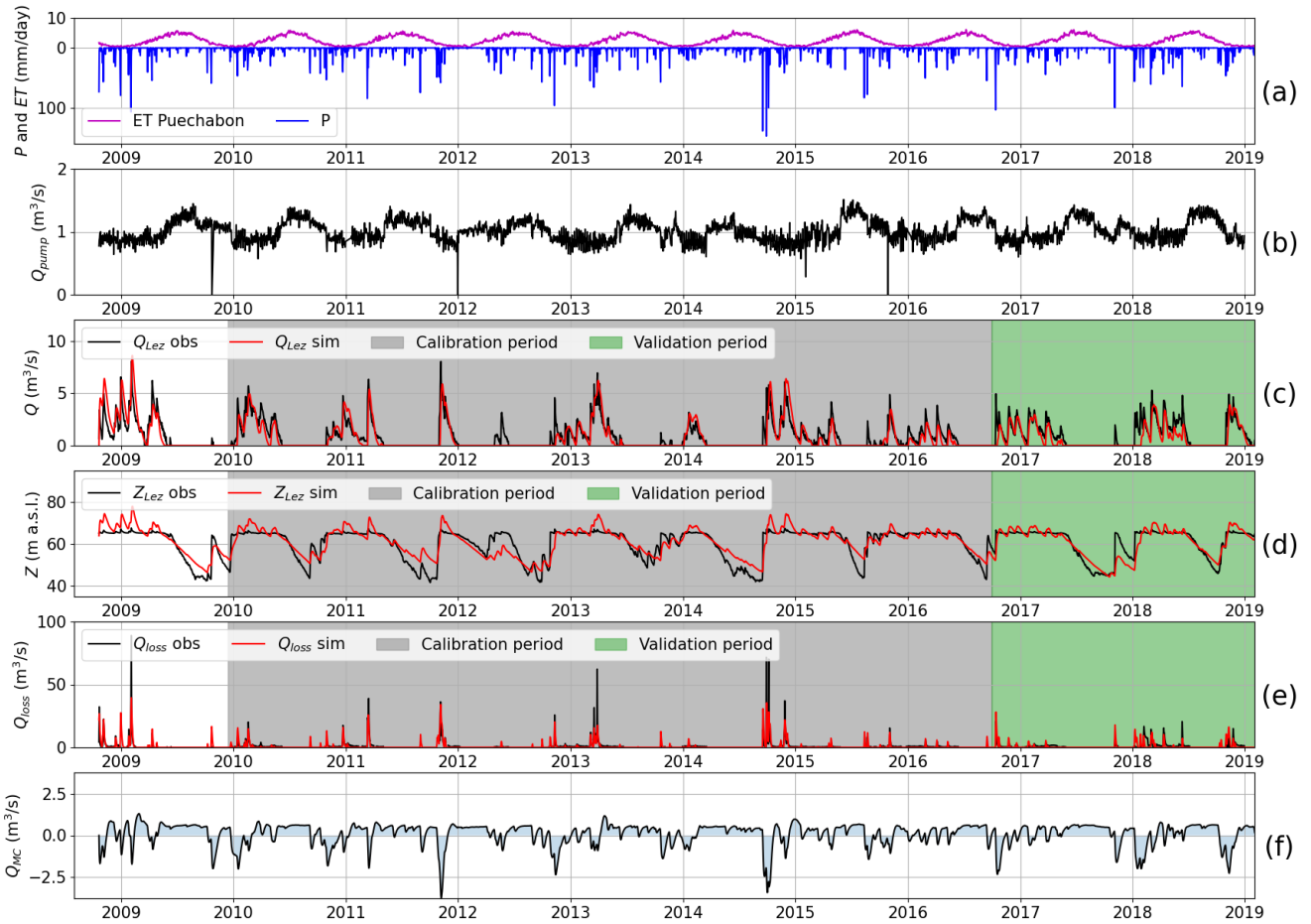
Figure 7. Daily time series for the Lez system: a) precipitations (P) and evapotranspiration (ET), b) groundwater abstraction (Q_{pump}), c) observed and simulated karst spring discharge (Q_{Lez} obs and Q_{Lez} sim), d) observed and simulated piezometric head (Z_{Lez} obs and Z_{Lez} sim), e) surface water discharge (Q_{loss}) and f) simulated exchanges fluxes between compartment M and C (Q_{MC}).

340   The available hydrological observations for model calibration consist of spring discharge Q_S, piezometric head measurement Z_C at the Lez spring and surface water discharge from secondary outlets and intermittent springs Q_{loss} (Figure 7, c, d and e). The surface water discharge is estimated as the difference in discharge measured at the Lavalette station (15 km downstream the Lez spring) and the discharge measured at the Lez spring, as proposed by Cousquer and Jourde (2022). Therefore, Q_{loss} includes all the water loss from the epikarst within several seasonal overflowing springs (i.e. Lirou spring, Restinclière spring

345   and Fleurette spring). KarstMod allows to easily handle with the various parameter estimation depending on the considered hydrological observations (i.e. spring discharge, piezometric head measurement, and surface discharge from the epikarst). The sampling procedure is set up to find n_{obj} = 5000 simulations with an aggregated objective function Φ greater than 0.6. As suggested by Cousquer and Jourde (2022), using complementary hydrological observations in addition to the spring discharge

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allows to reduce the parametric uncertainties in the modeling of the Lez spring discharge. Therefore, using a multi-objective calibration procedure implemented in KarstMod, the objective function is build such as:

$$\Phi = \frac{1}{3} \times NSE(Q_s) + \frac{1}{3} \times NSE(Z_C) + \frac{1}{3} \times NSE(Q_{loss}) \tag{4}$$

The calibration procedure leads to an optimal $\Phi = 0.65$ decomposed such as $\phi\,Q_s = 0.70$, $\phi\,Z_C = 0.57$ and $\phi\,Q_{loss} = 0.70$ within the calibration period. Model performance evaluation on the validation period shows suitable model performance for both spring discharge and piezometric with $\phi\,Q_s = 0.54$ and $\phi\,Z_C = 0.79$, but poor model performance according to the surface water discharge with $\phi\,Q_{loss} = 0.36$. Afterwards the results can be evaluated using the various features proposed in KarstMod (Figure 8). The results show higher model performances for Q_S and Z_C than for Q_{loss}. The model performance appears quite satisfactorily concerning the variable of interest to assess the impact of water management scheme on the groundwater resources within the Lez aquifer.

The simulated exchange fluxes between compartment M and C (Figure 7f) show consistent dynamics with the observations. Indeed, during periods of high flow the exchange fluxes are oriented from the compartment C to compartment M (i.e. Q_{MC} < 0). Significant precipitation events lead to rapid rises in piezometric head, saturation of the transmissive part of the aquifer and finally the establishment of overflow at the Lez spring (i.e. $Q_S > 0$) as well as the overflowing springs (i.e. $Q_{loss} > 0$). Conversely, during the periods of low piezometric head (i.e. both Q_S and Q_{loss} are nil), the simulated exchange fluxes are oriented from compartment M to compartment C (i.e. $Q_{MC} > 0$). Such flow exchanges between capacitive and transmissive part of karst aquifers has been evidenced using KarstMod on other karst environment (Sivelle et al., 2019; Duran et al., 2020; Frank et al., 2021; Labat et al., 2022).
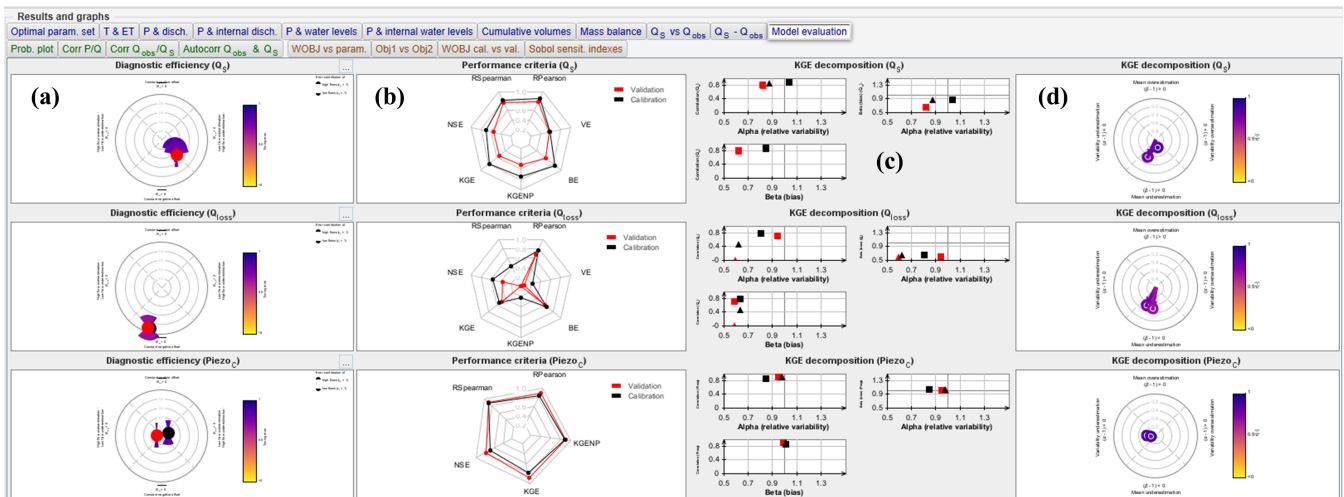
Figure 8. Screenshot of KarstMod with a focus on the sub-panel "Model evaluation". Application for the model evaluation on the Lez system. The panel is composed such as (i) each row correspond to the variable for calibration (Q_S, Q_{loss} and Piezo$_C$) and (ii) each column corresponds to (a) diagnostic efficiency plot, (b) radar plots, one should note that VE and BE are not computed according to the piezometric time series, (c) decomposition of KGE (square) and $KGENP$ (triangle) and (d) radar plot of the KGE decomposition.

5 Conclusions

KarstMod consists in a useful tool for the assessment of karst groundwater variability and sensitivity to anthropogenic pressures (e.g. groundwater abstraction). This tool is devoted to promote good practices in hydrological modeling for learning and occasional users. KarstMod requires no programming skills and offers a user friendly interface allowing any user to easily handle hydrological modeling. As a first step, KarstMod can be used to explore the ability of conceptual representations to explain observations such as discharge or piezometric heads in karst systems. A more advanced use of KarstMod is also possible as it provides a complete framework for (i) primary analysis of the data, (ii) comparison of various model structures, (iii) evaluation of the hydrological model performance as well as (iv) first assessment of parametric uncertainties. The research community increasingly uses KarstMod to address various challenges in karst hydrology, from understanding hydrological processes to practical applications such as evaluation of groundwater management plan, or even assessment of the impact of groundwater abstraction and climate changes on karst groundwater resources.

Future developments of KarstMod might include: (i) the consideration of land cover land use (LCLU) to consider the spatial heterogeneity in recharge processes (Sivelle et al., 2022a), (ii) the simulation of electrical conductivity (Chang et al., 2021), major ions concentration (Hartmann et al., 2013) or natural tracer such as air excess (Sivelle et al., 2022b), and (iii) the assessment of structural uncertainty (Cousquer et al., 2022). KarstMod should tend toward an open-source research software to avoid duplication of efforts in karst hydrological modeling. Also, a Python version is required for a better connection with additional framework for sensitivity analysis such as SAFE toolbox (Pianosi et al., 2015) and for model calibration

procedure such as particle swarm optimization (Eberhart and Kennedy, 1995; Lee, 2014). Finally, the development of the
385   KarstMod modeling platform will benefit better transparency and repeatability with an open-source approach, as observed on
other numerical tools (Pianosi et al., 2020).

Appendix A: Snow routine

Figure A1 shows the general workflow implemented in the snow routine. Psr^* (liquid water leaving the routine) is estimated
for each time step t based on the precipitation P and air temperature T time series for each sub-catchment. The total snow
390   routine output Psr is calculated as a weighted sum of Psr^* time series:

$$Psr = \sum_{i}^{N} Psr_i^* \times p_i \tag{A1}$$

where p_i is the proportion of the sub-catchment i regarding the complete catchment area such as $\sum p_i = 1$, and N is total
number of sub-catchments.

The snow routine requires four parameters, whose values are the same for all sub-catchments: the snowmelt temperature
395   threshold Ts [°C], the melt factor MF [L T^{-1} °C^{-1}], the refreezing factor CFR [-], and the water holding capacity of snow
CWH [-]. The snow routine allows estimating Psr^* according to the algorithm A1.
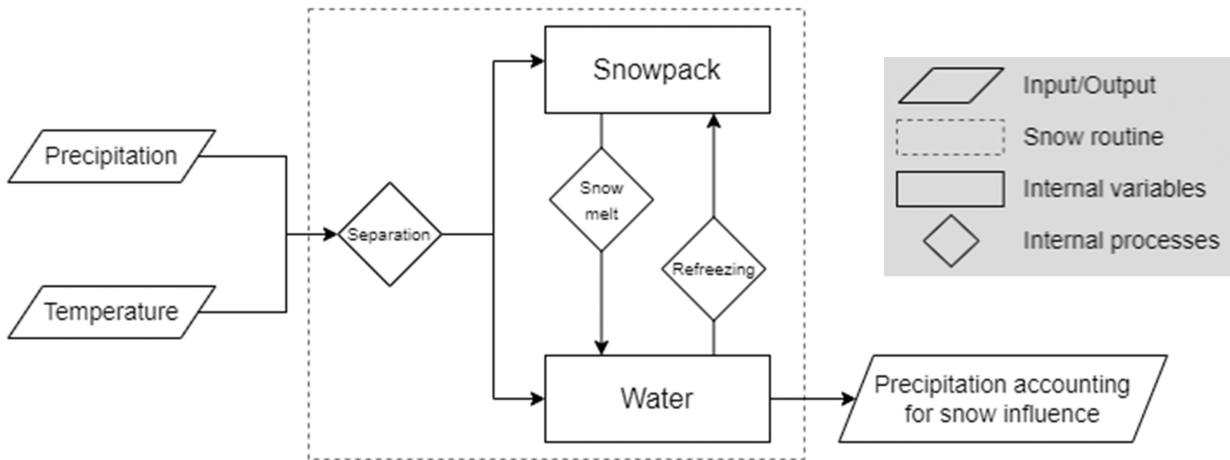
Figure A1. Snow routine workflow.

Algorithm A1 Estimating Psr^* in sub-catchment

With Psr^* = water leaving the routine/recharge to the soil (mm/dt), T_a = active temperature for snowmelt (°C), T_n = active temperature for refreezing (°C), m = snow melt (mm/dt), rfz = refreezing (mm/dt), v = solid component of snowpack depth (mm), vl = liquid component of snowpack depth (mm), and dt = temporal resolution.

for $t=1$ **to** t_{max} **do**
    $m[t] = min(MF \times T_a[t], v[t])$ *with* $T_a[t] = T[t] - T_s$
    $rfz[t] = min(CFR \times MF \times T_n[t], vl[t])$ *with* $T_n[t] = T_s - T[t]$
    $v[t+dt] = v[t] - m[t] + snow[t] + rfz[t]$
    if $vl[t+dt] > CWH \times v[t+dt]$ **then**
        $Psr^*[t] = vl[t+dt] - CWH \times v[t+dt]$
        $vl[t+dt] = CWH \times v[t+dt]$
    else
        $Psr^*[t] = 0$
    end
end

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