1	A physically based distributed karst hydrological model (QMG
2	model-V1.0) for flood simulation
3	Ji Li ^{1,*} , Daoxian Yuan ^{1,2} , Fuxi Zhang ³ , Jiao Liu ⁴ , Mingguo Ma ¹
4	¹ Chongqing Jinfo Mountain Karst Ecosystem National Observation and Research
5	Station, Chongqing Key Laboratory of Karst Environment, School of Geographical
6	Sciences, Southwest University, Chongqing 400715, China
7	² Key Laboratory of Karst Dynamics, MNR & Guangxi, Institute of Karst Geology,
8	Chinese Academy of Geological Sciences, Guilin 541004, China
9	³ College of Engineering Science and Technology, Shanghai Ocean University;
10	Shanghai Engineering Research Center of Marine Renewable Energy 201306, China
11	⁴ Chongqing municipal hydrological monitoring station, Chongqing 401120, China
12	Corresponding author: Ji Li (445776649@qq.com)
13	Abstract Karst trough and valley landforms are prone to flooding, primarily because of the
14	unique hydrogeological features of karst landforms, which are conducive to the spread of
15	rapid runoff. Hydrological models that represent the complicated hydrological processes in
16	karst regions are effective for predicting karst flooding, but their application has been
17	hampered by their complex model structures and associated parameter sets, especially for
18	distributed hydrological models, which require large amounts of hydrogeological data.
19	Distributed hydrological models for predicting flooding are highly dependent on distributed
20	modelling processes, complicated boundary parameter settings, and extensive
21	hydrogeological data processing steps, which are time consuming and computationally
22	expensive. In this study, a distributed physically based karst hydrological model called the

23 QMG (Qingmuguan) model is proposed. The structural design of this model is relatively 24 simple, and it is generally divided into surface and underground double-layered structures. 25 The parameters that represent the structural functions of each layer have clear physical meanings, and fewer parameters are required than are need for other distributed models. This 26 27 approach allows karst areas to be modelled with only a small amount of necessary hydrogeological data. Eighteen flood processes associated with the karst underground river 28 in the Qingmuguan karst trough valley are simulated by the QMG model, and the simulated 29 values agree well with observations, for which the average value of the Nash-Sutcliffe 30 31 coefficient is 0.92. A sensitivity analysis shows that the infiltration coefficient, permeability 32 coefficient, and rock porosity are the most important parameters in model calibration and optimization. The improved predictions of karst flooding obtained with the proposed QMG 33 34 model enhance the mechanistic understanding of runoff generation and flow in karst trough valleys. 35

36 Keywords: Simulation and forecasting of karst floods; Karst trough valleys; QMG
37 (Qingmuguan) model; Parametric optimization; Parameter sensitivity analysis

38 1 Introduction

Karst trough and valley landforms are very common in China, especially in the southwest. In 39 40 general, these karst areas are water scarce during most of the year because their surfaces 41 store very little rainfall, but they are also potential sources of floods because the local trough and valley landforms and topographic features facilitate the formation and propagation of 42 43 floods (White, 2002; Li et al., 2021). The coexistence of drought and flood is a typical 44 phenomenon in these karst trough and valley areas. For example, in the present study area, 45 the Qingmuguan karst trough valley, floods were historically prevalent during the rainy season. In recent years, with more extreme rainfall events and the increased area of 46

47 construction land in the region, rainfall infiltration has decreased, and rapid runoff over 48 impervious surfaces has increased, resulting in frequent catastrophic flooding in the basin 49 (Liu et al., 2009). Excess water flows from karst sinkholes and underground river outlets 50 during floods (Jourde et al., 2007, 2014; Martinotti et al., 2017), flooding large areas of 51 farmland and residential areas and causing serious economic losses (Gutierrez, 2010; Parise, 52 2010; Yu et al., 2020). Therefore, it is both important and urgent to simulate and predict 53 karst flooding events in karst trough and valley regions, such as the study area.

Hydrological models can be effective for forecasting floods and evaluating water 54 resources in karst areas (Bonacci et al., 2006; Ford and Williams, 2007; Williams, 2008, 55 56 2009). However, modelling floods in karst regions is extremely difficult because of the 57 complex hydrogeological structures of these regions. Karst water-bearing systems consist of 58 multiple media and are influenced by complex karst development dynamics (Worthington 59 et al., 2000; Kovács and Perrochet, 2008; Gutierrez, 2010), such as karst caves, conduits, 60 fissures and pores; thus, such systems are usually highly spatially heterogeneous (Chang and Liu, 2015; Teixeiraparente et al., 2019). In addition, the complex surface hydrogeological 61 62 conditions and the hydrodynamic conditions inside karst water-bearing media result in significant temporal and spatial differences in the hydrological processes in karst areas 63 64 (Geyer et al., 2008; Bittner et al., 2020).

In early studies of flood forecasting in karst regions, simplified lumped hydrological 65 models were commonly used to describe the rainfall-discharge relationship (e.g., Kovács 66 and Sauter, 2007; Fleury et al., 2007b; Jukić and Denić, 2009; Hartmann et al., 2014a). With 67 the development of physical exploration technology and the progress made in mathematics, 68 69 computing and other interdisciplinary disciplines, the level of modelling has gradually 70 improved (Hartmann and Baker, 2017; Hartmann, 2018; Petrie et al., 2021). Subsequently, 71 distributed hydrological models have been widely used in karst areas. The main difference 72 between lumped and distributed hydrological models is that the latter divide the entire basin into many subbasins to simulate runoff generation and confluence characteristics, thereby 73 effectively describing the physical properties of the hydrological processes that occur in 74 75 karst water-bearing systems (Jourde et al., 2007; Hartmann, 2018; Epting et al., 2018).

76 Because of their simple structure and low demand for modelling data, lumped 77 hydrological models have been used widely in karst areas (Kurtulus and Razack, 2007; 78 Ladouche et al., 2014). In a lumped model, a river basin is considered as a whole when 79 simulating runoff generation and flow paths, and there is no division into subbasins (Dewandel et al., 2003; Bittner et al., 2020). Lumped models usually consider the inputs and 80 outputs of the study area (Liedl and Sauter, 2003; Hartmann and Bake, 2013, 2017). In 81 82 addition, most of the model parameters are not optimized in a lumped model, and the 83 physical meaning of each parameter may be unclear (Chen, 2009; Bittner et al., 2020).

84 Distributed hydrological models are of high interest in flood simulation and forecasting 85 research (Ambroise et al., 1996; Beven and Binley, 2006; Zhu and Li, 2014). Compared with 86 lumped models, distributed models provide clear physical meaning regarding the model structure and mechanisms (Meng and Wang, 2010; Epting et al., 2018). In a distributed 87 88 hydrological model, an entire karst basin can be divided into many subbasins (Birk et al., 2005) using high-resolution digital elevation map (DEM) data. In the rainfall-runoff 89 90 algorithm of a model, the hydrogeological conditions and karst aquifer characteristics can be fully considered to precisely simulate runoff generation and flow processes (Martinotti et 91 92 al.,2017; Gang et al., 2019). Additionally, some basin-scale distributed hydrological models 93 (not specific groundwater numerical models, such as MODFLOW) have been applied in 94 karst areas, and they include the SHE/MIKE SHE model (Abbott et al., 1986a,b; Doummar 95 et al., 2012), the SWMM model (Peterson and Wicks, 2006; Blansett and Hamlett, 2010; 96 Blansett, 2011), TOPMODEL (Ambroise et al., 1996; Suo et al., 2007; Lu et al., 2013; Pan, 97 2014) and the SWAT model (Peterson and Hamlett, 1998; Ren, 2006).

98 The commonly used distributed hydrological models have various structures and 99 numerous parameters (Lu et al., 2013; Pan, 2014), and a model may require vast amounts of 100 data to build a framework for simulations in karst regions. For example, the distributed 101 groundwater model MODFLOW-CFPM1 requires detailed data regarding the distribution of 102 karst conduits in a study area (Reimann et al., 2009). Another example is the Karst–Liuxihe 103 model (Li et al., 2019); notably, there are fifteen parameters and five underground vertical 104 structures in the model. Such a complex structure increases the data demand, and modelling in karst areas is extremely difficult. In addition, a special borehole pumping test may be
 required to obtain the rock permeability coefficient.

107 To overcome the large data demands of distributed hydrological models in karst areas, a new 108 physically based distributed hydrological model-known as the QMG (Qingmuguan) 109 model-V1.0-was developed in the present study. Other commonly used karst groundwater 110 models with complex structures and parameters, such as the aforementioned 111 MODFLOW-CFPM1 model, require considerable hydrogeological data for modelling in 112 karst areas (Qin and Jiang, 2014). The new QMG model has high potential for application in 113 karst hydrological simulation and forecasting; it has certain advantages related to its 114 framework and structural design, such as a double-layer structure and few parameters. The 115 horizontal structure is divided into river channel units and slope units, and the vertical 116 structure below the surface is divided into shallow karst aquifer and deep karst aquifer 117 systems. This relatively simple model structure reduces the demand for modelling data in karst areas, and limited hydrogeological data are needed for modelling. To ensure that the 118 119 QMG model works well in karst flood simulation and prediction despite its relatively simple 120 structure and few parameters, we carefully designed the algorithms for runoff generation and 121 flow in the model. Additionally, to verify the applicability of the QMG model in flood 122 simulation in karst basins, we selected the Qingmuguan karst trough valley in Chongqing, 123 China, as the study area for flood simulation and uncertainty analysis. In particular, we analysed the sensitivity of the model parameters. 124

125 2 Study area and data

126 **2.1 Landform and topography**

127 The Qingmuguan karst trough valley is located in the southeastern part of the Sichuan Basin, 128 China, at the junction of the Beibei and Shapingba districts in Chongqing, with the 129 coordinates 29°40′N–29°47′N and 106°17′E–106°20′E. The basin covers an area of 130 13.4 km² and is part of the southern extension of the anticline at Wintang Gorge in the 131 Jinyun Mountains, with the anticlinal axis of Qingmuguan located in a parallel valley in eastern Sichuan (Yang et al., 2008). The surface of the anticline is heavily fragmented, and
faults are extremely well developed with large areas of exposed Triassic carbonate rocks.
Under the long-term erosion of karst water, a typical karst trough landform has formed,
which looks like a pen-holder structure, means 'three ridges with two troughs' (Liu et al.,
2009). This karst trough landform provides ideal conditions for flood propagation, and the
development of karst landforms is extremely common in this karst region of Southwest
China, especially in the karst region of Chongqing.

139 The basin is oriented in a narrow band of slightly curved arcs and is ~12 km long from 140 north to south. The direction of the mountains in the region is generally consistent with the 141 direction of the tectonic line. The map in Figure 1 gives an overview of the Qingmuguan 142 karst basin.

143

Figure 1. The Qingmuguan karst basin.

144 **2.2 Hydrogeological conditions**

145 The Qingmuguan basin is located within the subtropical humid monsoon climate zone, with an average temperature of 16.5°C and an average precipitation of 1250 mm concentrated 146 mainly from May-September. An underground river system has developed in the karst 147 trough valley, with a length of 7.4 km, and the water supply of the underground river is 148 149 mainly rainfall recharge (Zhang, 2012). Most of the precipitation collects in hillslope areas 150 and flows into the karst depressions at the bottom of the trough valley, where it provides recharge to the underground river through dispersed infiltration via surface karst fissures and 151 152 sinkholes (Fig. 1a). An upstream surface river forms in a gentle valley and enters the 153 underground river through the Yankou sinkhole (elevation 524 m). Surface water in the 154 middle and lower reaches of the river system enters the underground river system mainly 155 through cover-collapse sinkholes (Gutierrez et al., 2014) and fissures.

The stratigraphic and lithological characteristics of the basin are dominated largely by carbonate rocks of the Lower Triassic Jialingjiang Group (T_{1j}) and Middle Triassic Leikou Slope Group (T_{2l}) on both sides of the slope, with some quartz sandstone and mudstone outcrops of the Upper Triassic Xujiahe Group (T_{3xj}) (Zhang, 2012). The topography of the basin presents a general anticline (Fig. 1b), where carbonate rocks on the surface are corroded and fragmented and have high permeability. Compared with the core of the anticline, the shale of the anticline is less eroded and forms a good waterproof layer.

163 To investigate the distribution of karst conduits in the underground river system, we 164 conducted a tracer test in the study area. The tracer was placed into the Yankou sinkhole and 165 recovered in the Jiangjia spring (Fig. 1a,c). According to the tracer test results (Gou et al., 166 2010), the karst water-bearing medium in the aquifer was anisotropic, the karst conduits in 167 the underground river were extremely well developed, and there was a large single-channel 168 underground river approximately five metres wide. The response of the underground river to 169 rainfall was very fast, with the peak flow observed at the outlet of Jiangjia spring 6–8 h after rainfall based on the tracer test results. The flood peak rose quickly, and the duration of the 170 171 peak flow was short. The underground river system in the study area is dominated by large 172 karst conduits, which are not conducive to water storage in water-bearing media but are very 173 conducive to the propagation of floods.

174 2.3 Data

175 To build the QMG model to simulate karst flood events, the necessary modelling 176 baseline data had to be collected, and they included 1) high-resolution DEM data and 177 hydrogeological data (e.g., the thickness of the epikarst zone, rainfall infiltration coefficient for different karst landforms, and permeability coefficient of rock); 2) land use and soil type 178 179 data; and 3) rainfall data in the basin and water flow data for the underground river. The 180 DEM data were downloaded from a free internet database and had an initial spatial 181 resolution of 30×30 m. The spatial resolution of the land use and soil type data was 1000 182 \times 1000 m, and these data were also downloaded from the internet. After considering the applicability and computational strength of the model, as well as the size of the basin in the 183 study area (13.4 km²), the spatial resolution of the three types of data was resampled 184 uniformly in the QMG model and downscaled to 15×15 m based on the spatial discrete 185 method proposed by Berry et al. (2010). 186

The hydrogeological data necessary for modelling were obtained in three simple ways. 187 1) A basin survey was conducted to obtain the thickness of the epikarst zone, which was 188 189 achieved by observing the rock formations on hillsides following cutting for road 190 construction. Information was collected regarding the location, general shape, and size of karst depressions and sinkholes, and these data were combined with DEM data and used to 191 determine the convergence process of these depressions. The sinkholes in the basin are 192 cover-collapse sinkholes (Gutierrez et al., 2014) according to the basin survey. There are 3 193 large sinkholes (more than 3 metres in diameter) and 12 small sinkholes (less than 1 metre in 194 diameter). The rest of the sinkholes, 5 in total, are between 1 and 3 metres in diameter. The 195 196 confluence calculations for sinkholes in the model were based on the results of a previous study (Meng et al., 2009). 2) Empirical equations developed for similar basins were used to 197 obtain the rainfall infiltration coefficient for different karst landforms and the permeability 198 coefficient of rock. For example, the rock permeability coefficient was calculated based on 199 200 an empirical equation established based on a pumping test in a coal mine in the study area 201 (Li et al., 2019, 2022). 3) A tracer experiment was conducted in the study area (Gou et al., 202 2010) to obtain information on the underground flow direction and flow velocity; for instance, underground karst conduits are well developed in the area, and an underground 203 204 river approximately five metres wide is present. There is no hydraulic connection between 205 the underground river system in the area and the adjacent basin, which means that there is no 206 overflow recharge.

207 Rainfall and flood data are important model inputs and represent the driving factors of 208 hydrological models. In the study area, rainfall data were acquired with two rain gauges 209 located in the basin (Fig. 1a). Point rainfall was then spatially interpolated to obtain 210 basin-level rainfall (for such a small basin area, the rainfall results obtained from two rain 211 gauges were considered representative). There were 18 karst flood events from 14 April 2017 to 10 June 2019. We built a rectangular open channel at the underground river outlet 212 213 and set up a river gauge in the channel (Fig. 1a) to record the water level and flow data every 15 minutes. 214

215 **3 Methodology**

230

216 **3.1 Hydrological model framework and algorithms**

The hydrological model developed in this study was named the QMG model after the basin for which it was developed and to which it was first applied, i.e., the Qingmuguan basin. The QMG model has a two-layer structure, including a surface part and an underground part. The surface part mainly performs the runoff generation and surface routing calculations, and the underground part performs the routing calculations for the underground river system.

222 The structure of the QMG model is divided into a two-layer structure with horizontal 223 and vertical components. The horizontal structure of the model is divided into river channel 224 units and slope units. The vertical structure below the surface is divided into a shallow karst 225 aquifer (including soil layers, karst fissures and conduit systems in the epikarst zone) and a 226 deep karst aquifer system (bedrock and underground river system). With this relatively 227 simple model structure, only a small amount of hydrogeological data is needed in karst 228 regions. Figure 2 shows a flowchart of the modelling and calculation procedures required for 229 the QMG model.

Figure 2. Modelling flow chart of the QMG (Qingmuguan) model.

231 To accurately show the runoff generation and routing processes at the grid scale, the 232 karst subbasins are further divided into many karst hydrological response units (KHRUs) based on the high-resolution $(15 \times 15 \text{ m})$ DEM data in the model. The specific steps 233 234 involved in the division were adopted by referring to a study of hydrological response units 235 (HRUs) in TOPMODEL by Pan (2014). As the smallest basin units for computing, KHRUs 236 can effectively mitigate the spatial differences in karst development within units and reduce 237 the uncertainty in the classification of model units. Figure 3 shows the spatial structure of 238 the KHRUs.

Figure 3. Spatial structure of karst hydrological response units (KHRUs) (Li et al., 2021).

240 The right-hand side of Figure 3 shows a three-dimensional spatial model of KHRUs 241 established in the laboratory to visually reflect the storage and movement of water in a karst 242 water-bearing medium with spatial anisotropy and to provide technical support for establishing the hydrological model.

The modelling and operation of the QMG model involve three main stages: 1) spatial interpolation and the establishment of rainfall and evaporation calculations; 2) runoff generation and routing calculations for the surface river; and 3) routing calculations for underground runoff, including in the shallow karst aquifer and the underground river system.

248 **3.1.1 Rainfall and evaporation calculations**

In the QMG model, the spatial interpolation of rainfall is accomplished with a kriging method using ArcGIS 10.2 software. In some cases, the Thiessen polygon method may be a simpler method for rainfall interpolation if the number of rainfall gauges in the basin is sufficient. The point rainfall observed with the two rainfall gauges in the basin (Fig. 1a) was interpolated spatially into areal rainfall for the entire basin.

Basin evapotranspiration in the KHRUs was mainly from vegetation, the soil and water surfaces. These evapotranspiration components were calculated using the following equations (modified from Li et al., 2020):

257
$$\begin{cases} E_{v} = V^{'^{+\Delta t}} - V^{t} - P_{v} \\ E_{s} = \lambda E_{p}, \text{ if } F = F_{c} \\ E_{s} = \lambda E_{p} \frac{F}{F_{c}}, \text{ if } F < F_{\text{sat}} \\ E_{w} = \Delta e \cdot \left[1.12 + 0.62 \left(\Delta T \right)^{0.9} \right] \cdot \left[0.084 + 0.24 \left(1 - \gamma^{2} \right)^{1/2} \right] \cdot \left[0.348 + 0.5 \omega^{1.8 - 1.137 \omega^{0.05}} \right] \end{cases}$$
(1)

where E_{v} [mm] is the vegetal discharge, $V^{+\Delta v} - V^{t}$ [mm] is the rainfall variation due 258 259 to vegetation interception, P_{y} [mm] is the interception of rainfall by vegetation and E_{s} [mm] is the actual soil evaporation. The term λ is the evaporation coefficient. The term 260 261 E_p [mm] is potential evaporation, which can be measured experimentally or estimated with a water surface evaporation equation for E_{w} . The term F [mm] is the actual soil 262 moisture, F_{sat} [mm] is the saturation moisture content, F_c [mm] is the field capacity, E_w 263 264 [mm/d] is the evaporation from a water surface and $\Delta e = e_0 - e_{150}$ [hPa] is the draught head between the saturation vapour pressure of a water surface and the air vapour 265 pressure 150 m above the water surface. The term $\Delta T = t_0 - T_{150}$ [°C] is the temperature 266

267 difference between a water surface and a location 150 m above the water surface, γ is 268 the relative humidity 150 m above the water surface and ω [m/s] is the wind speed 269 150 m above the water surface.

270 3.1.2 Runoff generation

271 In the QMG model, the surface runoff generation in river channel units is associated with the rainfall in the basin that enters the river system after subtracting evaporation losses. This 272 273 portion of the runoff is directly involved in the routing process through the river system 274 rather than undergoing infiltration. In contrast, the process of runoff generation in slope units 275 is more complex and related to the developmental characteristics of the surface karst 276 features in the basin, the rainfall intensity and soil moisture. For example, when the soil is 277 saturated, there is the potential for excess infiltration-based surface runoff in exposed karst 278 slope units. Surface runoff generation in river channel units and slope units in KHRUs can 279 be described by the following equations (modified from Chen, 2009, 2018; Li et al., 2020):

280
$$\begin{cases} P_r(t) = \left[P_i(t) - E_p \right] \frac{L \cdot W_{\text{max}}}{A} \\ R_{\text{si}} = (P_i - f_i), P_i \ge f_{\text{max}} \\ R_{\text{si}} = 0, P_i < f_{\text{max}} \\ f_{\text{max}} = \alpha (F_c - F)^{\beta} + F_s \end{cases}$$
(2)

where $P_r(t)$ [mm] is the net rainfall (subtracting evaporation losses) in the river channel units at time t [h], $P_i(t)$ [mm] is the rainfall in the river channel units, L [m] is the length of the river channel, W_{max} [m] is the maximum width of the river channel selected and A [m²] is the cross-sectional area of the river channel. R_{si} [mm] is the excess infiltration runoff in the QMG model when the vadose zone is nonsaturated. Notably, the infiltration capacity f_{max} varies in different karst landform units. α and β are the parameters of the Holtan model, and F_s [mm] is the stable depth of soil water infiltration.

In the KHRUs (Fig. 3), underground runoff is generated primarily from the infiltration of rainwater and direct confluence recharge from sinkholes or karst windows. In the QMG model, underground runoff is calculated by the following equations (modified from Chen, 2018):

292
$$\begin{cases} R_g = R_0 \exp(-pt^m) \\ R_e = v_e \cdot I_w \cdot z \end{cases}$$
(3)

293 where

294
$$\begin{cases}
\frac{\partial R_e}{\partial x} + I_w \cdot z \cdot \frac{\partial F}{\partial t} = R_r - R_{epi} \\
v_e = K \cdot \tan(\alpha), \quad F > F_c \\
v_e = 0, \quad F \le F_c
\end{cases}$$
(4)

Here, R_g [mm] is the underground runoff depth (this part of underground runoff is mainly 295 296 directly from karst sinkholes or karst windows in the study area), R_0 [mm] is the average 297 depth of underground runoff, p and m are attenuation coefficients that were calculated by 298 conducting a tracer test in the study area, R_e [L/s] is the underground runoff generated from 299 rainfall infiltration in the epikarst zone, I_w [mm] is the width of the underground runoff zone 300 in the KHRUs, z [mm] is the thickness of the epikarst zone, R_r [mm²/s] is the runoff-based recharge in the KHRUs during period t, R_{epi} [mm²/s] is the water infiltration from rainfall, 301 302 v_e [mm/s] is the flow velocity of underground runoff, K [mm/s] is the permeability coefficient and α is the hydraulic gradient of underground runoff. If the soil moisture level 303 is less than the field capacity, $F \leq F_{c}$, and the vadose zone is not yet full, there will be no 304 305 underground runoff generation, and rainfall infiltration will fill the vadose zone before it 306 becomes saturated, at which point runoff is generated.

307 3.1.3 Channel routing and convergence

In the QMG model, runoff routing in KHRUs includes the confluence of the surface river channel and underground runoff. There are already many classic algorithms available for performing runoff routing calculations in river channel units and slope units, such as the Saint-Venant equations and Muskingum convergence model. In this study, the Saint-Venant equations were adopted to assess flow routing for the surface river and in hill slope units, and a wave movement equation was adopted for convergence calculations in slope units (Chen, 2009):

315
$$\begin{cases} \frac{\partial Q}{\partial x} + L \frac{\partial h}{\partial t} = q\\ S_f - S_0 = 0 \end{cases}$$
(5)

316 where

317
$$Q = vhL = \frac{L}{n}h^{\frac{5}{3}}S_0^{\frac{1}{2}}$$
(6)

318 Here, we customized two variables *a* and *b*:

319
$$\begin{cases} a = (\frac{n}{L}S_0^{-\frac{1}{2}})^{\frac{3}{5}} \\ b = \frac{3}{5} \end{cases}$$
(7)

Equation (7) was substituted into Eq. (5) and discretized with a finite-difference method,
yielding

322
$$\begin{cases}
\frac{\partial Q}{\partial x} + abQ^{(b-1)}\frac{\partial Q}{\partial t} - q = 0 \\
\frac{\Delta t}{\Delta x}Q_{i+1}^{t+1} + a(Q_{i+1}^{t+1})^b = \frac{\Delta t}{\Delta x}Q_i^{t+1} + a(Q_{i+1}^t)^b + q_{i+1}^{t+1}\Delta t
\end{cases}$$
(8)

323 The Newton–Raphson method was used for the iterative calculation using Eq. (8):

324
$$\left[Q_{i+1}^{t+1}\right]^{k+1} = \left[Q_{i+1}^{t+1}\right]^{k} - \frac{\frac{\Delta t}{\Delta x} \left[Q_{i+1}^{t+1}\right]^{k} + a\left(\left[Q_{i+1}^{t+1}\right]^{k}\right)^{b} - \frac{\Delta t}{\Delta x} Q_{i}^{t+1} - a\left(Q_{i+1}^{t}\right)^{b} - q_{i+1}^{t+1}\Delta t}{\frac{\Delta t}{\Delta x} + ab\left(\left[Q_{i+1}^{t+1}\right]^{k}\right)^{b-1}}$$
(9)

325 where Q [L/s] is the convergence of water flow in slope units, L [dm] is the width of the 326 runoff zone in a slope unit, h [dm] is the runoff depth and q $[dm^2/s]$ is the lateral inflow in the KHRUs. Here, the friction slope S_f equals the hill slope S_0 , and the inertia term and 327 328 the pressure term in the motion equation of the Saint-Venant equation set were ignored. The term v [dm/s] is the flow velocity of surface runoff in the slope units, as calculated by the 329 Manning equation. Additionally, *n* is the roughness coefficient of the slope units, Q_i^{t+1} [L/s] 330 is the slope inflow in a KHRU at time t+1 and Q_{i+1}^{t+1} [L/s] is the slope discharge in the 331 332 upper adjacent KHRU at time t+1.

333 Similarly, surface river channel convergence was described based on the Saint-Venant 334 equations, and a diffusion wave movement equation was adopted; therefore, the inertia term 335 in the motion equation was ignored:

336
$$\begin{cases} \frac{\partial Q}{\partial x} + \frac{\partial A}{\partial t} = q\\ S_f = S_0 - \frac{\partial h}{\partial x} \end{cases}$$
(10)

A finite-difference method and the Newton–Raphson method were used to iteratively solvethe above equation set:

339
$$\begin{cases} \left[Q_{i+1}^{t+1} \right]^{k+1} = \left[Q_{i+1}^{t+1} \right]^{k} - \frac{\Delta t}{\Delta x} \left[Q_{i+1}^{t+1} \right]^{k} + c \left(\left[Q_{i+1}^{t+1} \right]^{k} \right)^{b} - \frac{\Delta t}{\Delta x} Q_{i}^{t+1} - c \left(Q_{i+1}^{t} \right)^{b} - q_{i+1}^{t+1} \Delta t \\ \frac{\Delta t}{\Delta x} + c b \left(\left[Q_{i+1}^{t+1} \right]^{k} \right)^{b-1} \end{cases}$$
(11)
$$c = \left(\frac{1}{3600} n \chi^{\frac{2}{3}} S_{f}^{-\frac{1}{2}} \right)^{\frac{3}{5}} \end{cases}$$

where Q [L/s] is the water flow in surface river channel units, A [dm²] is the cross-sectional area of discharge, c is a custom intermediate variable and χ [dm] is the wetted perimeter of the discharge cross-section.

343 The underground runoff area in the model includes the convergence region of the 344 epikarst zone and underground river. In the epikarst zone, the karst water-bearing media are 345 highly heterogeneous (Williams, 2008). For example, anisotropic karst fissure systems and 346 conduit systems consist of corrosion fractures. When rainfall infiltrates into the epikarst 347 zone, water moves slowly through the small (less than 10 cm in this study) karst fissure 348 systems, and it flows rapidly in larger (more than 10 cm) conduits. The key to estimating the flow velocity lies in determining the width of karst fractures. In the KHRUs (Fig. 3), a 349 350 fracture width of 10 cm was used as a threshold value (Atkinson, 1977) based on a borehole 351 pumping test in the basin. Thus, if the fracture width exceeded 10 cm, then the water 352 movement in the fracture was defined as rapid flow; otherwise, it was defined as slow flow. 353 The flow in the epikarst zone was calculated by the following equation (modified from Beven and Binley, 2006): 354

355
$$Q(t)_{ijk} = b_{ijk} \cdot \frac{\Delta h}{\Delta l} R_i C_j \cdot T(t)_{slow/rapid}$$
(12)

356 where

357
$$\begin{cases} T(t)_{\text{slow}} = nr \frac{\rho g R_i C_j L_k}{12\nu} \\ T(t)_{\text{rapid}} = \frac{K_{ij} \left(e^{-f_{ij} h_{ij}} - e^{-f_{ij} z_{ij}} \right)}{f_{ij}} \end{cases}$$
(13)

Here, $Q(t)_{ijk}$ [L/s] is the flow in the epikarst zone at time t, b_{ijk} [dm] is the width of the runoff zone, $\frac{\Delta h}{\Delta l}$ is the dimensionless hydraulic gradient, $T(t)_{slow/rapid}$ is the dimensionless hydraulic conductivity, ρ [g/L] is the density of water, g [m/s²] is gravitational acceleration, n is the number of valid computational units, $R_i C_j L_k$ [L] is the volume of the ijk-th KHRU, v is the kinematic viscosity coefficient, f_{ij} is the attenuation coefficient in the epikarst zone, h_{ij} [dm] is the depth of shallow groundwater and z_{ij} [dm] is the thickness of the epikarst zone.

The distinction between rapid and slow flows in the epikarst zone is not absolute. Notably, the established fracture threshold of 10 cm may be underrepresentative because pumping tests were conducted in only five boreholes in the region. In fact, there is usually water exchange between the rapid and slow flow zones at the junctions of large and small fissures in karst aquifers. In the QMG model, this water exchange can be described with the following equation (modified from Li et al., 2021):

371
$$\begin{cases} Q = \alpha_{i,j,k} \left(h_n - h_{i,j,k} \right) \\ \alpha_{i,j,k} = \sum_{ip=1}^{np} \frac{\left(K_w \right)_{i,j,k} \pi d_{ip} \frac{1}{2} \left(\Delta l_{ip} \tau_{ip} \right)}{r_{ip}} \end{cases}$$
(14)

Here, $\alpha_{i,j,k}$ [dm²/s] is the water exchange coefficient in the *ijk*-th KHRU, $(h_n - h_{i,j,k})$ [dm] is the water head difference between the rapid and slow flow zones at the junction of large and small fissures in KHRUs, *np* is the number of fissure systems connected to the adjacent conduit systems, $(K_w)_{i,j,k}$ [dm/s] is the permeability coefficient at the junction of a fissure and conduit, d_{ip} and r_{ip} [dm] are the conduit diameter and radius, respectively ΔI_{ip} [dm] is the length of the connection between conduits *i* and *p*, and τ_{ip} is the conduit curvature. Some of the parameters in this equation, such as $(K_w)_{i,j,k}$ and $(h_n - h_{i,j,k})$, were obtained by conducting an infiltration test in the study area.

The convergence patterns in the underground river system have an important influence on the flow regime at the basin outlet. To facilitate the routing calculations in the QMG model, the underground river system can be generalized into large multiple-conduit systems. During floods, these conduit systems are mostly under pressure. Whether the water flow is laminar or turbulent depends on the flow regime at that time. The water flow into these conduits is calculated based on the Hagen–Poiseuille equation and the Darcy–Weisbach equation (Shoemaker et al., 2008):

387
$$\begin{cases} Q_{\text{laminar}} = -A \frac{gd^2 \partial h}{32 v \partial x} = -A \frac{\rho gd^2 \Delta h}{32 \mu \tau \Delta l} \\ Q_{\text{turbulent}} = -2A \sqrt{\frac{2gd |\Delta h|}{\Delta l \tau}} \log \left(\frac{H_c}{3.71d} + \frac{2.51v}{d\sqrt{\frac{2gd^3 |\Delta h|}{\Delta l \tau}}} \right) \frac{\Delta h}{|\Delta h|} \end{cases}$$
(15)

Here, Q_{laminar} [L/s] is the laminar flow in the conduit systems, A [dm²] is the conduit cross-sectional area, d [dm] is the conduit diameter, ρ [kg/dm³] is the density of water, $v=\mu/\rho$ is the coefficient of kinematic viscosity, $\Delta h/\tau\Delta l$ is the hydraulic slope of the conduits, τ is the dimensionless conduit curvature, $Q_{\text{turbulent}}$ [L/s] is the turbulent flow in the conduit systems and H_c [dm] is the average conduit wall height.

393 3.2 Parameter optimization

394 In total, the QMG model has 12 parameters, of which flow direction and slope are 395 topographic parameters that can be determined from the DEM without parametric optimization, and the remaining 10 parameters require calibration. Other distributed
hydrological models with multiple structures usually have many parameters. For example,
the Karst–Liuxihe model (Li et al., 2021) has 15 parameters that must be calibrated. In the
QMG model, each parameter is normalized as

$$x_i = x_i^* / x_{i0}, (16)$$

where x_i is the dimensionless parameter value for *i* after it is normalized, x_i^* is the 401 parameter value for *i* in actual physical units, and x_{i0} is the initial or final value of x_i . 402 403 Through the processing of Eq. (16), the value range of the model parameters is limited to a hypercube $K_n = (X \mid 0 \le x_i \le 1, i = 1, 2, ..., n)$, and K is a dimensionless value. This 404 405 normalization process ignores the influence of the spatiotemporal variation in the underlying 406 surface attributes on the parameters while also simplifying parameter classification and the 407 number of model parameters to a certain extent. Accordingly, the model parameters can be further divided into rainfall-evaporation parameters, epikarst zone parameters and 408 409 underground river parameters. Table 1 lists the parameters of the QMG model.

410 **Table 1.** Parameters of the QMG model.

Because the QMG model has relatively few parameters, it is possible to calibrate them manually, which is easy and does not require a special program for parameter optimization. However, the disadvantage is that this manual approach is subjective, which can lead to uncertainty in the manual parameter calibration process. To compare the effects of parameter optimization on model performance, both manual parameter calibration and the improved chaotic particle swarm optimization algorithm (IPSO) were used for the automatic calibration of model parameters, and the effects of both on flood simulation were compared.

In general, the structure and parameters of a standard particle swarm optimization algorithm (PSO) are simple, with the initial parameter values obtained at random. For parameter optimization in high-dimensional multipeak hydrological models, the standard PSO is easily limited to local convergence and cannot achieve the optimal effect, and the late evolution of the algorithm may also cause problems, such as premature convergence or stagnant evolution, due to the 'inert' aggregation of particles, which seriously affects the efficiency of parameter selection. It is necessary to overcome the above problems so that the algorithm can converge to the global optimal solution with a high probability. In parameter optimization for the QMG model, we improved the standard PSO algorithm by adding chaos theory and developed the IPSO method; notably, 10 cycles of chaotic disturbances were added to improve the activity of the particles. The inverse mapping equation for the chaotic variable is

430
$$\begin{cases} X_{ij} = X_{\min} + (X_{\max} - X_{\min}) * Z_{ij} \\ Z'_{ij} = (1 - \alpha) Z^* + \alpha Z_{ij} \end{cases}$$
(17)

431 where X_{ij} is the optimization variable for the model parameters, $(X_{max} - X_{min})$ is the 432 difference between the maximum and minimum values of X_{ij} , Z_{ij} is the variable before the 433 disturbance is added, Z_{ij} is the chaotic variable after a disturbance is added, α is a variable 434 determined by the adaptive algorithm ($0 \le \alpha \le 1$), and Z^* is the chaotic variable formed when 435 the optimal particle is mapped to the interval [0,1]. The flowchart of IPSO is shown in 436 Figure 4.

437

Figure 4. Algorithm flow chart of IPSO.

438 **3.3 Uncertainty analysis**

Uncertainties in hydrological model simulation results usually originate from three factors: the input data, the model structure and the model parameters (Krzysztofowicz, 2014). In the present study, the input data (e.g., rainfall, flood and hydrogeological data) were first validated and preprocessed based on observations to reduce uncertainty.

Second, we simplified the structure of the QMG model to reduce the structural uncertainty. As a mathematical and physical model, a hydrological model is characterized by some uncertainty in flood simulation and forecasting because of the errors in the system structure and selected algorithm (Krzysztofowicz and Kelly, 2000). The model in this study was designed with full consideration of the relationship between the amount of data required to build the model and model performance in flood simulation and forecasting in karst regions. The entire model framework was integrated through simple structures and easy-to-implement algorithms based on the concept of distributed hydrological modelling. Conventionally, the level of uncertainty increases with the growing complexity of the model structure. We therefore ensured that the structure of the QMG model was simple when it was designed, and the double-layer model was divided into surface and underground structures to reduce structural uncertainty.

Third, we focused on analysing the uncertainty and sensitivity of model parameters and the applied optimization method; specifically, a multiparametric sensitivity analysis method (Choi et al., 1999; Li et al., 2020) was used to analyse the sensitivity of the parameters in the QMG model. The steps in the parameter sensitivity analysis are as follows.

459 1) Selection of the appropriate objective function

The Nash–Sutcliffe coefficient is widely used to evaluate the performance of hydrological models (Li et al., 2020, 2021); therefore, it was used to assess the QMG model in this study. Because the most important factor in flood forecasting is the peak discharge, it is used in the Nash coefficient equation:

$$NSC = 1 - \frac{\sum_{i=1}^{n} (Q_i - Q_i)^2}{\sum_{i=1}^{n} (Q_i - \overline{Q})^2},$$
(18)

where *NSC* is the Nash–Sutcliffe coefficient, Q_i [L/s] is the observed flow discharge, Q_i' [L/s] is the simulated discharge, \overline{Q} [L/s] is the average observed discharge and *n* [h] is the observation period.

468 2) Parameter sequence sampling

464

The Monte Carlo sampling method was used to sample 8000 groups of parameter sequences. The parametric sensitivity of the QMG model was analysed and evaluated by comparing the differences between the a priori and a posteriori distributions of the parameters.

473 3) Parameter sensitivity assessment

The a priori distribution of a model parameter is its probability distribution, and the a posteriori distribution refers to the conditional distribution calculated after sampling, which can be calculated based on the results of parameter optimization. If there is a significant difference between the a priori distribution and the a posteriori distribution of a parameter, then the parameter being tested is characterized by high sensitivity; conversely, if there is no obvious difference, then the parameter is insensitive. The a priori distribution of a parameter is calculated as

481
$$\begin{cases} P_{i,j}(NSC_{i,j} \ge 0.85) = \frac{n}{N+1} \times 100 \\ \sigma_i = \sum_{j=1}^n \left(P_{i,j} - \overline{P_{i,j}}\right)^2 \end{cases}$$
(19)

where P_{ij} is the probability associated with a given a priori distribution when 482 $NSC_{i,j} \ge 0.85$. We used a simulated Nash coefficient of 0.85 as the threshold value, and n 483 was the number of occurrences of a Nash coefficient greater than 0.85 in flood simulations. 484 485 In each simulation, only a certain parameter was changed, and the remaining parameters 486 remained unchanged. If the Nash coefficient of a simulation exceeded 0.85, then the flood simulation results were considered acceptable. The term σ_i is the difference between an 487 acceptable value and the overall mean, which represents the parametric sensitivity 488 $(0 < \sigma_i < 1)$. The higher the σ_i value is, the more sensitive the parameter. In this study, N 489 denotes the 8000 parameter sequences, and $\overline{P_{i,j}}$ is the average value of the a priori 490 distribution. 491

492 **3.4 Model settings**

After the model was built and before it was run, some of the initial conditions, such as the basin division scheme, the initial soil moisture levels, and the initial parameter ranges, were set. 1) In the study area, the entire Qingmuguan karst basin was divided into 893 KHRUs, including 65 surface river units, 466 hill slope units, and 362 underground river units. The division of these units formed the basis for runoff generation and convergence calculations. 2) The initial soil moisture level was set to 0–100% of the saturated moisture

content in the basin, and the specific soil moisture level before each flood was determined 499 500 through a trial calculation. 3) The hydraulic head boundary conditions for the groundwater 501 zone were determined by a tracer test in the basin, and a perennial stable water level in area adjacent to the groundwater divide was used as the fixed head value at the model boundary. 502 The base flow of the underground river was determined to be 35 L/s based on the perennial 503 average dry season runoff. 4) The ranges of initial parameters and the convergence 504 conditions were set before parameter optimization (Figure 4). 5) Parameter optimization and 505 506 flood simulation were performed to validate the performance of the QMG model in karst 507 basins.

508 4 Results and discussion

509 4.1 Parameter sensitivity results

510 The number of parameters in a distributed hydrological model is generally large, and it 511 is important to perform a sensitivity analysis of each parameter to quantitatively assess the 512 impact of the different parameters on model performance. In the QMG model, each 513 parameter was divided into four categories according to its sensitivity: (i) highly sensitive, 514 (ii) sensitive, (iii) moderately sensitive, and (v) insensitive. In the calibration of model 515 parameters, insensitive parameters do not need to be calibrated, which can greatly reduce the 516 number of calculations and improve the efficiency of model operations.

517 The flow process in the calibration period (14 April to 10 May 2017) was adopted to 518 calculate the sensitivity of the model parameters, and calculations were based on 519 equation (19). The parameter sensitivity results are listed in Table 2.

520

Table 2 Parametric sensitivity results for the QMG model.

In Table 2, the value of σ_i [equation (19)] represents a parameter's sensitivity, and the higher the value is, the more sensitive the parameter. The results in Table 2 indicate that the rainfall infiltration coefficient, rock permeability coefficient, rock porosity, and parameters related to the soil water content, such as the saturated water content and field capacity, are sensitive parameters. The order of parameter sensitivity is as follows: infiltration coefficient > permeability coefficient > rock porosity > specific yield > saturated water content > field 527 capacity > flow direction > thickness > slope > soil coefficient > channel roughness >
528 evaporation coefficient.

529 In the QMG model, parameters are classified as highly sensitive, sensitive, moderately 530 sensitive, and insensitive according to their influence on the flood simulation results. In Table 4, we divide the sensitivity of model parameters into four levels based on the σ_i value: 531 1) highly sensitive parameters, $0.8 < \sigma_i < 1$; 2) sensitive parameters, $0.65 < \sigma_i < 0.8$; 3) 532 moderately sensitive parameters, $0.45 < \sigma_i < 0.65$; and 4) insensitive parameters, 533 $0 < \sigma_i < 0.45$. The highly sensitive parameters are the infiltration coefficient, permeability 534 coefficient, rock porosity, and specific yield. The sensitive parameters are the saturated 535 water content, field capacity, and thickness of the epikarst zone. The moderately sensitive 536 parameters are the flow direction, slope, and soil coefficient. The insensitive parameters are 537 538 channel roughness and the evaporation coefficient.

539 4.2 Parametric optimization

In total, the QMG model includes 12 parameters, of which only eight need to be optimized, which is relatively few for distributed models. The flow direction and slope, as channel roughness and the evaporation coefficient, which are insensitive parameters, need not be calibrated; this approach can improve the convergence efficiency of the model parameter optimization process.

In the study area, 18 karst floods from 14 April 2017 to 10 June 2019 were recorded at 545 the underground river outlet to validate the effects of the QMG model in karst hydrological 546 547 simulations. The calibration period was 14 April to 10 May 2017 at the beginning of the 548 flow process, with the remainder of the period used as the validation period. In the QMG 549 model, the IPSO algorithm was used to optimize the model parameters. To demonstrate the 550 need for parameter optimization for the distributed hydrological model, the flood simulation 551 results obtained using the initial parameters of the model (without parameter calibration) and 552 the optimized parameters were compared. Figure 5 shows the iterative parameter optimization process for the QMG model. 553

Figure 5 Iterative parameter optimization process.

554

555 Figure 5 shows that almost all parameters considerably fluctuate at the beginning of the 556 optimization, and after approximately 15 iterative optimization calculations, most of the 557 linear fluctuations become significantly less variable, which indicates that the algorithm 558 tends to converge (possibly only locally). When the number of iterations exceeded 25, all 559 parameters remain essentially unchanged, suggesting that the algorithm converged (at this 560 point, global convergence was achieved). It took only 25 iterations to achieve definite convergence for parameters in the applied IPSO algorithm; thus, this approach is extremely 561 562 efficient in terms of parameter optimization for distributed hydrological models. In previous 563 studies of the optimization of the parameters of the Karst-Liuxihe model in similar basin 564 areas, 50 iterative steps were required to reach convergence in automatic parameter 565 optimization (Li et al., 2021), demonstrating the effectiveness of the IPSO algorithm.

566 To evaluate the effect of parameter optimization, the convergence efficiency of the 567 algorithm and, more importantly, the parameters after calibration were assessed in flood 568 simulation cases. Figure 6 shows the flood simulation results.

569 Figure 6 Flow simulation results of the QMG model based on parameter optimization.

570 Figure 6 shows that the flows simulated following parameter optimization were better 571 than those obtained with the initial model parameters. The simulated flow values based on 572 the initial parameters were relatively small, with the simulated peak flows being notably smaller than the observed values; additionally, there were large errors between the simulated 573 and observed values. In contrast, the simulated flows produced by the QMG model after 574 parameter optimization were very similar to the observed values, which indicates that 575 calibration of the model parameters was necessary and that there was an improvement in 576 parameter optimization achieved through the use of the IPSO algorithm in this study. In 577 578 addition, the flow simulation effect was better in the calibration periods than in the 579 validation periods (Fig. 6).

580 To compare the results of the flow process simulations with the initial model parameters 581 and the optimized parameters, six evaluation indices (Nash–Sutcliffe coefficient, correlation

coefficient, relative flow process error, flood peak error, water balance coefficient, and peak
time error) were applied in this study, and the results are presented in Table 3.

584

Table 3 Flood simulation evaluation indices following parametric optimization.

Table 3 shows that the evaluation indices of the flood simulations after parameter 585 586 optimization were better than those obtained with the initial model parameters. The average values of the initial parameters for these six indices were 0.81, 0.74, 27%, 31%, 0.80, and 587 588 5 h, respectively. For the optimized parameters, the average values were 0.90, 0.91, 16%, 589 14%, 0.94, and 3 h, respectively. The flood simulation effects after parameter optimization 590 clearly improved, implying that parameter optimization for the QMG model is necessary and 591 that the IPSO algorithm for parameter optimization is an effective approach that can greatly 592 improve the convergence efficiency of parameter optimization and ensure that the model 593 performs well in flood simulations.

594 **4.3 Model validation in flood simulations**

595 Following parameter optimization, we simulated the whole flow process (14 April 2017 to 10 June 2019) based on the optimized and initial parameters of the QMG model (Fig. 6). 596 597 This approach allowed us to visually assess a long series of flow processes obtained with the 598 model. To reflect the simulation effect of the model for different flood events, we divided the 599 whole flow process into 18 flood events and then used the initial parameters of the model 600 and the optimized parameters to verify the model performance in flood simulations. Figure 7 and Table 4 show the flood simulation effects and the calculated evaluation indices using 601 602 both the initial and optimized parameters.

603

Figure 7 Flood simulation effects based on the initial and optimized parameters.

604

Table 4 Flood simulation indices for model validation.

Figure 7 shows that the flood simulation values obtained using the initial parameters were smaller than the observed values, and the model performance improved in flood simulations after parameter optimization. The simulated flood processes were in good agreement with observations, and flood peak flows were especially well simulated. From the flood simulation indices in Table 4, the average water balance coefficient based on the initial parameters was 0.69, i.e., much less than 1, indicating that the simulated water in the model was unbalanced. After parameter optimization, the average value was 0.92, indicating that parameter optimization had a significant impact on the water balance calculation.

Table 4 shows that the average values of the six indices (Nash-Sutcliffe coefficient, 613 614 correlation coefficient, relative flow process error, flood peak error, water balance coefficient, and peak time error) for the initial parameters were 0.79, 0.74, 26%, 25%, 0.69, 615 616 and 5 h, respectively, while for the optimized parameters, the average values were 0.92, 0.90, 10%, 11%, 0.92, and 2 h, respectively. All evaluation indices improved after parameter 617 618 optimization, with the average values of the Nash coefficient, correlation coefficient, and 619 water balance coefficient increasing by 0.13, 0.16, and 0.23, respectively. Additionally, the 620 average values of the relative flow process error, flood peak error, and peak time error decreased by 15%, 14%, and 3 h, respectively. These reasonable flood simulation results 621 622 confirmed that parameter optimization with the IPSO algorithm was necessary and effective for the QMG model. 623

624 Compared with the overall flow process simulation shown in Figure 6, each flood process was better simulated by the QMG model (Fig. 7). Notably, in the QMG model and 625 626 the applied algorithm, the main consideration is flood process calculations, and the correlation algorithm for dry-season runoff was not sufficiently described. For example, 627 628 equations (12)–(15) are used in the flood convergence algorithm. Consequently, the model is 629 not good at simulating other flow processes, such as dry-season runoff, leading to low accuracy in simulations of the overall flow process. The next phase of our research will 630 focus on refining the algorithm related to dry-season runoff and improving the 631 632 comprehensive performance of the model.

633 4.4 Uncertainty analysis

634 **4.4.1 Assessment and reduction of uncertainty**

In general, the uncertainty in model simulation is due mainly to three factors: (i) the uncertainty of input data, (ii) the uncertainty of the model structure and algorithm and (iii) the uncertainty of the model parameters. In the practical application of a hydrological model, 638 these three uncertainties are usually interwoven, which leads to overall uncertainty in the 639 final simulation results (Krzysztofowicz, 2014). Therefore, this study focused on the 640 uncertainties in the input data, the model structure and the parameters to reduce the overall 641 uncertainty of the simulation results.

642 First, the input data-mainly rainfall-runoff data and hydrogeological data-were 643 preprocessed, which substantially reduced their uncertainty. Second, we simplified the 644 structure of the QMG model, with only two structural layers in the horizontal and vertical directions. This relatively simple structure greatly reduced the modelling uncertainty. In 645 646 contrast, our previous Karst-Liuxihe model (Li et al., 2021) included five layers, which led 647 to considerably uncertainty. Third, appropriate algorithms for runoff generation and 648 confluence were selected. In general, different models are designed for different purposes, 649 which leads to notable differences in the algorithms used. In the OMG model, most of the 650 rainfall-runoff algorithms used have been validated by the research results of others, and some of them were improved for karst flood simulation and forecasting with the QMG 651 652 model. For example, the algorithm for the generation of excess infiltration runoff [Eq. (2)] 653 was an improvement of the version used in the Liuxihe model (Chen, 2009, 2018; Li et al., 654 2020). Finally, the algorithm for parameter optimization was improved. Considering the 655 shortcomings of the standard PSO algorithm, which tends to converge locally, IPSO for 656 parameter optimization was developed in this study by adding chaotic perturbation factors. 657 The flood simulation results after parameter optimization were much better than those 658 obtained with the initial model parameters (Figs. 6 and 7 and Tables 2 and 3), which 659 indicates that parameter optimization is necessary for distributed hydrological models and 660 can reduce the uncertainty of model parameters.

661 4.4.2 Sensitivity analysis

The parameter sensitivity results in Table 2 show that the rainfall infiltration coefficient in the QMG model was the most sensitive parameter and was the key to the generation of excess infiltration surface runoff and the separation of surface runoff from subsurface runoff. If the rainfall infiltration coefficient is greater than the infiltration capacity, excess infiltration surface runoff will be generated on exposed karst landforms; otherwise, all rainfall will infiltrate into the vadose zone and then continue to seep into the underground river system, eventually flowing out of the basin through the underground river outlet. The flow modes of surface runoff and underground runoff were completely different, resulting in a large difference in the simulated flow results. Therefore, the rainfall infiltration coefficient had the greatest impact on the final flood simulation results.

Other highly sensitive parameters, such as the rock permeability coefficient, rock porosity and specific yield, were used as the basis for dividing between slow flow in karst fissures and rapid flow in conduits. The division of slow and rapid flows also had a considerable impact on the discharge at the outlet of the basin. Slow flow plays an important role in water storage in karst aquifers and is very important for the replenishment of river base flow in the dry season. Rapid flow in large conduit systems dominates flood runoff and is the main component of the flood water volume in the flood season.

679 Parameters related to the soil water content, including the saturated water content, field capacity and thickness, were sensitive parameters and had a large influence on the flood 680 681 simulation results. Notably, the soil moisture content prior to flooding affects how flood flows rise and when peaks occur. If the soil is already very wet or even saturated before 682 flooding, a flood will rise quickly and reach a peak, and the flood peak flow will be sharp 683 and short. This type of flood can easily occur and can lead to a disaster-causing flood event. 684 685 In contrast, if the soil in the basin is very dry before flooding, the rainfall will first saturate the vadose zone; then, the rainfall will infiltrate into the underground river. The flood peak at 686 687 the river basin outlet is therefore delayed.

The moderately sensitive parameters were the flow direction, slope and soil coefficient; they had a specific influence on the flood simulation results, but the influence was not as great as that of the highly sensitive and sensitive parameters. The insensitive parameters were channel roughness and the evaporation coefficient. The amount of water lost via evapotranspiration is very small compared to the total volume of flood water, and evapotranspiration was therefore the least-sensitive parameter in the QMG model.

694 **5** Conclusions

In this study, a new distributed physically based hydrological model, i.e., the QMG model, was proposed to accurately simulate floods in karst trough and valley landforms. The main conclusions of this paper are as follows.

698 The QMG model has high application potential in karst hydrology simulations. Other distributed hydrological models usually have multiple structures, resulting in the need for a 699 700 large amount of data to build models in karst areas (Kraller et al., 2014). The QMG model 701 has only a double-layer structure, with clear physical meaning, and a small amount of basic data, such as some necessary hydrogeological data, is needed to build the model in karst 702 areas. For example, the distribution and flow direction of underground rivers must be known 703 704 and can be inferred from tracer tests at low cost. There are fewer parameters in the QMG model than in other distributed hydrological models, with only 10 parameters that need to be 705 706 calibrated.

The flood simulations after parameter optimization were much better than those based on the initial model parameters. After parameter optimization, the average values of the Nash coefficient, correlation coefficient and water balance coefficient increased by 0.13, 0.16 and 0.23, respectively, and the average relative flow process error, flood peak error and peak time error decreased by 15%, 14% and 3 h, respectively. Parameter optimization is necessary for distributed hydrological models, and the improved IPSO algorithm in this study was effective.

In the QMG model, the rainfall infiltration coefficient I_c , the rock permeability coefficient *K*, the rock porosity R_p and the parameters related to the soil water content were sensitive parameters. The order of parameter sensitivity was infiltration coefficient > permeability coefficient > rock porosity > specific yield > saturated water content > field capacity > flow direction > thickness > slope > soil coefficient > channel roughness > evaporation coefficient.

This QMG model is suitable for karst trough and valley landforms, such as those in the study area, where the topography is conducive to the spread of flood water. In the future, it must be verified whether this model is applicable to other karst areas and landforms. In addition, although the studied basin area is very small, but the hydrological similarity among different small basin areas varies greatly (Kong and Rui, 2003). The size of the area to be modelled has a great influence on the choice of spatial resolution for modelling (Chen et al., 2017). Therefore, it must be determined whether the QMG model is suitable for flood forecasting in large karst basins.

728 Model development.

The QMG model presented in this study uses Visual Basic language programming. The 729 general framework of the model and the algorithm consist of three parts: the modelling 730 approach, the rainfall-runoff generation and convergence algorithm, and the parameter 731 732 optimization algorithm. As a free and open-source hydrological modelling program (QMG model-V1.0), we provide all modelling packages, including the model code, installation 733 734 package, simulation data package and user manual, free of charge. It is important to note that the model we provide is for scientific research purposes only and should not be used for any 735 736 commercial purposes (Creative Commons Attribution 4.0 International).

The model installation program can be downloaded from Zenodo and should be cited as (JI
LI. (2021, June 16). QMG model-V1.0. Zenodo. <u>http://doi.org/10.5281/zenodo.4964701</u> and
<u>http://doi.org/10.5281/zenodo.4964697</u>) (registration required). The user manual can be
downloaded from <u>http://doi.org/10.5281/zenodo.4964754</u>.

741 Code availability.

All codes for the QMG model-V1.0 in this paper are available and free, and the code can be
downloaded from Zenodo at <u>http://doi.org/10.5281/zenodo.4964709</u> (registration required)
(Cite as JI LI. (2021, June 16). QMG model-V1.0 code (Version v1.0). Zenodo).

745 **Data availability.**

All data used in this paper are available, findable, accessible, interoperable, and reusable.

The simulation data and modelling data package can be downloaded from <u>http://doi.org/10.5281/zenodo.4964727</u>. The DEM was downloaded from the Shuttle Radar Topography Mission database at <u>http://srtm.csi.cgiar.org</u>. The land use-type data were downloaded from <u>http://landcover.usgs.gov</u>, and the soil-type data were downloaded from <u>http://www.isric.org</u>. These data were last accessed on 15 October 2020.

752 Author contributions. JIL was responsible for the calculations and writing of the whole

753 paper. DY helped conceive the structure of the model. ZF and JL provided significant

- assistance in the English translation of the paper. MM provided flow data from the study
- 755 area.

756 Competing interests.

757 The authors declare that they have no conflicts of interest.

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982 Tables

Parameters	Variable name	Physical property
Infiltration coefficient	I_c	Meteorological
Evaporation coefficient	λ	Vegetation cover
Soil thickness	h	Karst aquifer
Soil coefficient	S_b	Soil type
Saturated water content	S_c	Soil type
Rock porosity	R_p	Karst aquifer
Field capacity	F_{c}	Soil type
Permeability coefficient	K	Karst aquifer
Flow direction	F_d	Landform
Slope	S_{0}	Landform
Specific yield	S_y	Karst aquifer
Channel roughness	n	Landform

983 Table 1 Parameters of the QMG model.

984 Table 2 Parametric sensitivity results in the QMG model.

I_c	λ	h	S_b	S_c	S_y	F_d	S_0	R_p	F_{c}	K	п
0.92	0.24	0.71	0.58	0.8	0.83	0.74	0.68	0.86	0.78	0.89	0.36

985 Table 3 Flood simulation evaluation index through parametric optimization.

Parameter optimization	Parameter types	Nash coefficient	Correlation coefficient	Relative flow process error/%	Flood peak error/%	Water balance coefficient	Peak time error (hours)
Calibration	Initial	0.82	0.77	24	29	0.82	4
periods	Optimized	0.91	0.94	14	12	0.95	2
Validation	Initial	0.79	0.71	29	32	0.77	6
periods	Optimized	0.88	0.87	18	16	0.92	3
Average	Initial	0.81	0.74	27	31	0.8	5
value	Optimized	0.9	0.91	16	14	0.94	3

986 Table 4 Flood simulation indices for model validation.

Floods	Parameter types	Nash coefficient	Correlation coefficient	Relative flow process error/%	Flood peak error/%	Water balance coefficient	Peak time error/(hours)
2017042408	Initial	0.77	0.7	28	29	0.71	-5
2017042408	Optimized	0.95	0.89	11	15	0.88	-2
2017050816	Initial	0.78	0.71	19	19	0.76	-4
2017030810	Optimized	0.92	0.88	11	9	0.94	-2
2017061518	Initial	0.76	0.6	25	32	0.63	-5

	Optimized	0.91	0.93	12	11	0.95	-3
2017071015	Initial	0.78	0.82	25	37	0.64	-4
2017071013	Optimized	0.92	0.87	8	7	0.94	-2
2017001512	Initial	0.81	0.62	21	16	0.78	-5
2017071312	Optimized	0.9	0.92	13	10	0.9	-4
2017100815	Initial	0.75	0.68	30	26	0.62	-2
2017100015	Optimized	0.94	0.86	11	15	0.92	-1
2018052016	Initial	0.78	0.68	25	21	0.67	5
2010032010	Optimized	0.91	0.93	10	13	0.94	2
2018060815	Initial	0.82	0.79	27	22	0.69	-6
2010000015	Optimized	0.9	0.92	11	12	0.93	-4
2018071212	Initial	0.84	0.75	26	24	0.61	5
20100/1212	Optimized	0.91	0.88	8	15	0.92	3
2018081512	Initial	0.71	0.78	26	24	0.78	-4
2010001312	Optimized	0.89	0.94	12	11	0.89	-3
2018090516	Initial	0.85	0.68	28	23	0.68	-5
2010070510	Optimized	0.93	0.87	12	10	0.92	-2
2018092514	Initial	0.79	0.78	23	19	0.59	5
2010072314	Optimized	0.88	0.88	9	11	0.89	2
2018101208	Initial	0.78	0.81	28	25	0.63	5
2010101200	Optimized	0.92	0.94	11	10	0.94	2
2018111208	Initial	0.79	0.81	25	24	0.65	-6
2010111200	Optimized	0.94	0.86	13	12	0.92	-2
2019042512	Initial	0.78	0.8	26	36	0.8	5
2017042512	Optimized	0.89	0.94	9	16	0.93	2
2019051513	Initial	0.84	0.77	32	27	0.79	4
2017031313	Optimized	0.91	0.88	9	13	0.95	2
2019052516	Initial	0.74	0.75	29	26	0.63	-5
2017032310	Optimized	0.92	0.86	7	15	0.96	-2
2019060518	Initial	0.85	0.83	28	25	0.78	-4
	Optimized	0.95	0.96	10	12	0.92	-2
Average	Initial	0.79	0.74	26	25	0.69	5
value	Optimized	0.92	0.9	10	11	0.92	2



1- stratigraphic boundary, 2- sinkhole, 3- karst depression, 4- underground river, 5- karst spring, 6- surface river, 7- river gauge, 8- rain gauge, and 9- geographical name
a. Qingmuguan karst basin (modified from Yu et al., 2016)





b. Lithologic cross section AA' of the Yankou sinkhole (modified from Zhang, 2012)





Figure 2 Modelling flowchart of the QMG (Qingmuguan) model.







Figure 5 Iterative process of parameter optimization.









