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# 1 An explainable deep learning model based on 2 hydrological principles for flood simulation and 3 forecasting

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7 **Abstract:** Deep learning (DL) models always perform well in hydrological simulation but lack physical-  
8 based principles. To address this gap, we integrate the runoff generation and flow routing principals of  
9 Xinanjiang (XAJ) model into the architecture of recurrent neural network (RNN) units and establish a  
10 physical-based XAJRNN neural network layer. Subsequently, this layer is fused with LSTM layers to  
11 construct an explainable deep learning (EDL) model, which underwent testing at the Lushui River and  
12 Qingjiang River basins in China. Compared to benchmark models, the proposed EDL model performs  
13 very well, the average Nash-Sutcliffe efficiency (*NSE*) values for these two basins are 0.98 and 0.94,  
14 respectively. The small flood peak relative errors (*PRE*) and peak timing difference ( $\Delta T$ ) close to zero  
15 demonstrate that the EDL model can accuracy simulate flood events. Notably, the EDL model not only  
16 enhances simulation accuracy over ordinary DL models but also enhances interpretability by  
17 incorporating physical principles, thereby offering fresh insights for the fusion of DL and hydrological  
18 models for flood simulation and forecasting.

## 19 1 Introduction

20 In the modern era, flood disasters present substantial threats to both human societies and the natural  
21 environment (Guido et al., 2023). With the intensification of global climate change and rapid  
22 urbanization, the accuracy and timeliness of flood forecasting have become increasingly important. Flood  
23 forecasting typically relies on hydrological models (Thaisiam et al., 2024). By analyzing the rainfall-  
24 runoff relationships from historical periods, hydrological models simulate hydrological processes within  
25 a watershed. Combining these with forecasted rainfall data, such models can forecast flow discharges,



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26 river water levels, and probabilities of flood occurrence. In recent years, advancements in computational  
27 power and artificial intelligence (AI) technologies have significantly improved the accuracy and real-  
28 time responsiveness of hydrological models (Hirabayashi et al., 2013), offering more scientific and  
29 efficient support for disaster prevention and mitigation efforts.

30 Traditional hydrological models often rely on statistical methods and empirical formulas; however,  
31 these approaches exhibit limitations when tackling complex and nonlinear hydrological processes (Roy  
32 et al., 2023). In recent years, deep learning (DL) technologies have made significant advancements in  
33 various fields, particularly in time series prediction, where they display strong potential. DL, a domain  
34 dedicated to uncovering patterns and extracting knowledge from large datasets, enables computers to  
35 autonomously learn algorithms, analyze extensive sample data, and identify patterns, facilitating  
36 predictions on unfamiliar data. This process closely aligns with hydrological modeling, which discerns  
37 patterns by analyzing historical hydrometeorological data, generalizing, and simulating hydrological  
38 processes. Consequently, DL has attracted widespread attention in hydrology (Nearing et al., 2021).

39 DL commonly refers to deep neural networks, a form of representational learning technique that  
40 links simple nonlinear computational units through multi-layer network architectures to understand  
41 intricate relationships. It falls within the realm of machine learning (ML) (Yann et al., 2015). The term  
42 "deep" in DL signifies network structures with multiple layers and neurons, although there is no precise  
43 definition of "deep." Generally, it denotes models that necessitate substantial data and encompass  
44 numerous layers and neurons. These layers convert their inputs into higher-level features, magnifying  
45 crucial factors for output variability while reducing irrelevant variations. This facilitates automatic  
46 feature extraction, contrasting with "shallow" networks or conventional ML algorithms that rely on  
47 expert knowledge and engineering skills for designing feature extractors. This is a key rationale behind  
48 the increasing application of DL models over shallow networks in recent years (Frank et al., 2020).  
49 Structurally, the standard recurrent neural network (RNN), exemplified by Long Short-Term Memory  
50 (LSTM), remains the foundational model architecture for deep learning-driven hydrological forecasting.  
51 As an RNN subset in DL, LSTM has gained prominence for its efficacy in managing sequential data and  
52 capturing long-term dependencies. LSTM tackles the challenges of vanishing and exploding gradients in  
53 traditional RNNs when handling lengthy sequences through gated mechanisms, resulting in superior



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54 performance in time-dependent prediction tasks (Hochreiter and Schmidhuber, 1997).

55 DL has been extensively utilized in various fields. In hydrology, where processes are not yet fully  
56 understood, it exhibits promise in identifying physical processes through a data-mining lens. However,  
57 achieving accurate predictions is not the sole aim. Hydrologists are interested in whether models are in  
58 line with fundamental physical principles, are interpretable, and contribute to scientific knowledge  
59 advancement. Traditional physics-based hydrological models generally provide better interpretability  
60 and physical consistency, relying less on data and complementing DL models. As a result, the fusion of  
61 physics-based mechanisms and data-driven models has garnered significant attention in recent years,  
62 showcasing potential in advancing scientific inquiry (Nearing et al., 2021; Shen, 2018). Currently, the  
63 coupling of DL and physics-based models focuses on four main aspects.

64 (1) Introducing physical mechanisms into DL models' loss functions

65 Worland et al. (2019) developed a multi-output multilayer perceptron (MLP) model to forecast flow  
66 duration curve (FDC) quantiles, incorporating FDC monotonicity constraints into the loss function. This  
67 approach resulted in forecasts that adhered to monotonicity and closely matched the FDC derived from  
68 observations. Wang et al. (2020) not only incorporated physical laws into the loss function but also  
69 integrated expert knowledge in the form of inequalities, constructing Theory-guided Neural Networks  
70 (TgNN). TgNN demonstrated superior predictive performance compared to standard DL models. Xie et  
71 al. (2021) encoded three physical conditions in rainfall-runoff forecasting into the loss function.  
72 Experiments across 531 Catchment Attributes and Meteorology for Large-sample Studies (CAMELS)  
73 basins showed improvements in the average Nash-Sutcliffe efficiency (*NSE*) from 0.52 to 0.61, enhanced  
74 peak flow simulating, and reduced unreasonable negative values. Pokharel et al. (2023) tested the effects  
75 of incorporating mass balance, energy balance, and storage-discharge relationships into the loss function  
76 of DL models across 34 basins, finding performance improvements in some basins, particularly with  
77 mass and energy balance constraints, which were effective in 38% and 32% of basins, respectively. Frame  
78 et al. (2023) concluded that strict adherence to the water balance principle might degrade forecasting  
79 performance due to data errors. DL models, which do not necessarily enforce the water balance principle,  
80 can accommodate data biases and outperform traditional hydrological models in runoff forecasting.

81 (2) Using DL models as post-processors



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82           Correcting errors in forecasting from physics-based models can significantly improve forecasting  
83 accuracy. Cho and Kim (2022) employed LSTM to learn correlations between meteorological data and  
84 WRF-Hydro forecast errors, applying this approach to calibrate WRF-Hydro forecasting. Experiments  
85 in South Korean basins showed *NSE* values reaching 0.95, compared to 0.72 before calibration. Similarly,  
86 Han and Morrison (2022) and Frame et al. (2021) applied LSTM to post-process multi-period forecasting  
87 from the National Water Model in the United States. Boucher et al. (2020) utilized the simulated runoff  
88 of the GR4J hydrological model and observed water temperature as inputs to construct an MLP model,  
89 demonstrating notable improvements compared to models without assimilation. Cui et al. (2021)  
90 proposed a novel EDL model combining the Xinanjiang (XAJ) hydrological model with LSTM for multi-  
91 step flood forecasting. This model used XAJ outputs as inputs to the LSTM, enhancing the physical  
92 mechanism of DL models.

93           (3) Using DL models to calibrate parameters in traditional hydrological models

94           Tsai et al. (2021) proposed a parameter learning method to calibrate HBV model parameters. The  
95 DL model generated parameters instead of directly outputting runoff, which were then combined with  
96 inputs to produce runoff through the physical model. Applying this method across 1,802 basins showed  
97 median Kling-Gupta Efficiency (*KGE*) values improving from 0.48 to 0.59 compared to calibration via  
98 evolutionary algorithms followed by parameter regionalization. Similarly, Feng et al. (2023, 2022), Shen  
99 et al. (2023) and Song et al. (2024) used DL models to calibrate HBV model parameters based on  
100 meteorological data and basin attributes, driving hydrological models to simulate runoff. In addition to  
101 the above calibration of lumped model parameters, a similar method is also used to calibrate the  
102 confluence model parameters. Zhong et al. (2024a, 2024b) used DL model to calibrate parameters in the  
103 Muskingum-Cunge method and construct a distributed physics-driven DL hydrological model. Bindas et  
104 al. (2024) introduced a novel differentiable routing method ( $\delta$ MC-JuniatahydroDL2) combining the  
105 Muskingum-Cunge routing model with neural networks to infer Manning's roughness and channel  
106 geometry parameters. The method provided more accurate long-term routing forecasts, especially in  
107 untrained sub-basins.

108           (4) Designing DL models based on physical mechanisms

109           Encoding rules directly into neural networks represents a direct fusion of physics-based and data-



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110 driven models. Hoedt et al. (2021) modified LSTM structures to enforce water balance over specific  
111 periods. Experiments across 531 CAMELS basins showed improved peak flow performance despite no  
112 overall improvement in *NSE*. Jiang et al. (2020) modified RNN structures to incorporate state variables  
113 (e.g., soil moisture) from EXP-HYDRO model as recurrent unit states, combining these with other neural  
114 network layers to construct a physics-guided RNN. Experiments in 671 CAMELS basins demonstrated  
115 median *NSE* improvements from 0.60 to 0.71, with reductions in peak flow bias and improved baseflow  
116 simulations. De la Fuente et al. (2024) proposed HydroLSTM, which models hydrological principles to  
117 enhance interpretability, achieving comparable performance to LSTM models while requiring fewer unit  
118 states. Similarly, Li et al. (2024) embedded EXP-HYDRO processes into RNN units, developing a  
119 process-driven DL model that enhanced process understanding of rainfall-runoff relationships.  
120 Experiments across 531 CAMELS basins demonstrated improvements over LSTM model. Wang et al.  
121 (2024) introduced a novel distributed hydrological modeling framework combining HydroPy distributed  
122 hydrological model principles encoded into RNN units and DL models to calibrate physical parameters,  
123 improving runoff and water volume simulations.

124       The current integration of DL models with physical mechanisms mainly involves loosely coupled  
125 approaches, such as modifying loss functions or calibrating parameters. Further exploration is needed to  
126 integrate physical hydrological mechanisms into neural network architectures, constructing models with  
127 strong physical consistency and superior forecasting performance to facilitate new hydrological insights.  
128 The novelty of study is using the runoff generation and flow routing principals of the XAJ model to  
129 establish a physical-based XAJRNN neural network layer within an ordinary RNN framework by  
130 identifying model state variables and fluxes under a differential equation. A EDL model combining the  
131 XAJRNN layer and LSTM is constructed and tested in the Lushui River and Qingjiang River basins to  
132 demonstrate the advantages of the EDL model in flood simulation. The findings may offer a novel  
133 pathway for integrating DL models with hydrological physical mechanisms to improve flood forecasting  
134 accuracy.

135       The rest of this paper is organized as follows. The case study and materials are introduced in Section  
136 2. Section 3 presents the methodologies. Section 4 evaluates and analyses the simulated results. Section  
137 5 discusses the strengths as well as the weaknesses of the proposed model. Conclusions and outlook are



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138 given in Section 6.

## 139 **2 Study area and data**

### 140 **2.1 Study basin**

#### 141 **(1) Lushui River basin**

142 The Lushui River is a primary tributary of the middle Yangtze River, with a basin area of  
143 approximately 3,950 km<sup>2</sup>. The basin's terrain slopes from high elevations in the southeast to lower areas  
144 in the northwest. The basin is located in a subtropical monsoon climate zone, characterized by warm and  
145 humid conditions, with an average annual temperature of approximately 15.5°C and an average annual  
146 rainfall of 1,550 mm. The Lushui River's annual runoff volume reaches 3.03 billion m<sup>3</sup>, with rainfall  
147 concentrated from May to September, accounting for 70% of the annual total. At the river valley's outlet,  
148 the Lushui Reservoir has a total storage capacity of approximately 408 million m<sup>3</sup>, with only 163 million  
149 m<sup>3</sup> allocated for flood control. In early July 1995, the reservoir experienced its largest flood event, with  
150 an inflow peak of 4,500 m<sup>3</sup>/s and a three-day runoff of 500 million m<sup>3</sup>. In 2017, six flood events occurred,  
151 with peak inflows exceeding 1,000 m<sup>3</sup>/s, reaching a maximum inflow of 4,400 m<sup>3</sup>/s (Cui et al., 2021;  
152 Xiang et al., 2024). The geographical location of Lushui Reservoir is shown in Figure 1.

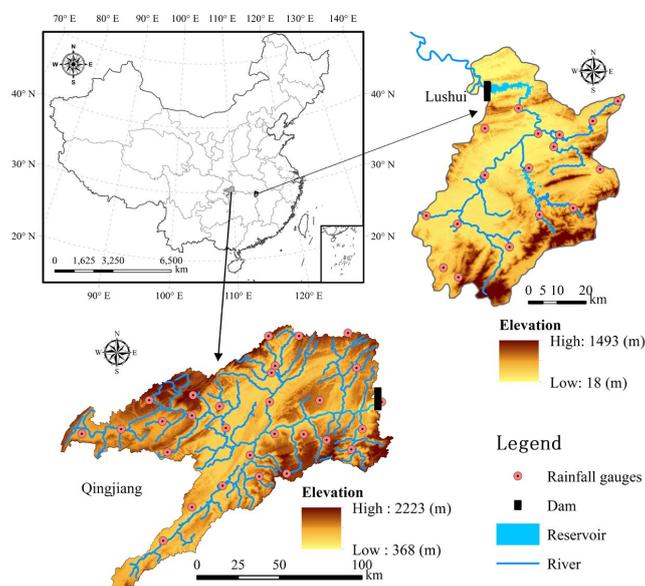
#### 153 **(2) Qingjiang River basin**

154 The Qingjiang River, a primary tributary of the Yangtze River in the middle reaches, has a basin  
155 area of approximately 17,000 km<sup>2</sup>. The region receives an average annual rainfall of 1,460 mm, with the  
156 majority falling between April and September, representing 75%–78% of the annual total. Situated in the  
157 heavy rainfall region of western Hubei Province, the basin's terrain facilitates the uplift of warm, moist  
158 air and is frequently affected by southwest cyclones. With a natural elevation drop of 1,430 m, the area  
159 features steep terrain and a high river gradient, leading to swift water flow convergence and significant  
160 fluctuations in flood levels. Consequently, the area is susceptible to severe rainfall and flood disasters.  
161 Along the main stream of the Qingjiang River, three sizable reservoirs exist, with the Shuibuya Reservoir  
162 serving as the central hub for the basin's cascade development, overseeing an area of roughly 10,860 km<sup>2</sup>.  
163 Located in Badong County, Hubei Province, the Shuibuya Reservoir plays a crucial role in the



164 hydropower development of the Qingjiang River. It greatly forms an integral component of the flood  
165 control system in the middle and lower reaches of the Yangtze River (Zhou et al., 2014). This study  
166 specifically focuses on the basin controlled by the Shuibuya Reservoir, as depicted in Figure 1.

167



168

169 **Figure 1: Sketch map of river networks and rainfall gauges in the Lushui River and Qingjiang River basins.**

## 170 2.2 Data

171 The study collected flood season data (Lushui River basin: May 1 to October 31, 2012–2019;  
172 Qingjiang River basin: April 1 to October 31, 2012–2020) that includes rainfall, pan evaporation, and  
173 inflow datasets. For Lushui River basin, 3 h rainfall data from 17 gauges, 3 h pan evaporation, and 3 h  
174 inflow discharge was collected. The data from 2012 to 2016 were used for training, and the data from  
175 2017 to 2019 for testing. For Qingjiang River basin, 6 h rainfall from 28 gauges, 6 h pan evaporation,  
176 and 6 h inflow discharge was gathered. The data from 2012 to 2016 were used for training, and the data  
177 from 2017 to 2020 for testing. The Thiessen polygon method was used to calculate the areal mean rainfall  
178 and pan evaporation for both basins.



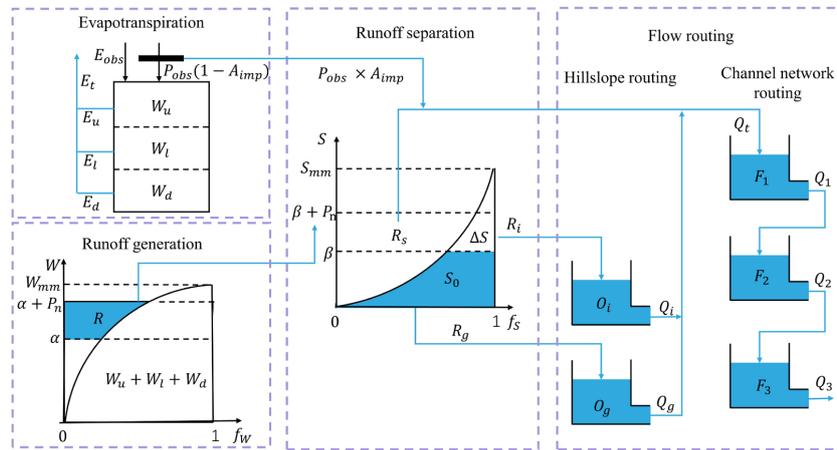
179 **3 Methodologies**

180 **3.1 XAJRNN neural network layer**

181 **3.1.1 XAJ model overview**

182 In this study, the evapotranspiration of the XAJ model uses a three-layer soil moisture model. The  
 183 runoff generation uses a tension water capacity curve (Zhao, 1992, 1993). In the runoff separation, the  
 184 runoff is divided into three types using the free water capacity curve: surface runoff, interflow runoff,  
 185 and groundwater runoff. The flow routing includes both hillslope routing and channel network routing  
 186 submodules, which use linear reservoirs and Nash unit hydrographs (Singh, 1977), respectively. The  
 187 logical structure of the XAJ model is shown in Figure 2.

188



189  
 190 **Figure 2: Structure diagram of the XAJ model.**

191 The model consists of input variables, state variables, fluxes, output variables, and parameters, along  
 192 with their corresponding mathematical equations. Input variables include areal mean rainfall and  
 193 measured pan evaporation, while the output variable is the simulated runoff. State variables represent  
 194 physical quantities that characterize the watershed's state, and their dimensions are independent of time  
 195 (La Follette et al., 2021). The state variables of the XAJ model are shown in Table A1. Fluxes describe  
 196 the exchange of water within the watershed or between the watershed and external environments. These  
 197 can be expressed as functions of state variables or other fluxes, and their dimensions are time-dependent



198 (La Follette et al., 2021). The fluxes of the XAJ model are shown in Table A2. The mathematical  
199 equations can be divided into state variable control equations and constitutive equations for fluxes. The  
200 control equations describe how state variables evolve over time, while the constitutive equations establish  
201 the relationships between unknown fluxes and state variables or known fluxes. Detailed information on  
202 the XAJ model is provided in Text A1.

### 203 3.1.2 Derivation of XAJRNN

204 Establishing the XAJ model in the watershed can be considered a complete system that represents  
205 changes in state variables within the watershed, such as the variation in the average tension water storage  
206 of the upper soil layer. At the same time, the XAJ model also describes how the watershed system  
207 responds to specific input conditions. These responses can be expressed through a combination of  
208 ordinary differential equations (ODE) and output equations:

$$209 \begin{cases} \frac{d}{dt}h(t) = F(h(t), x(t); \varphi_f) \\ y(t) = G(h(t), x(t); \varphi_g) \end{cases} \quad (1)$$

210 where:  $h(t)$  represents the state variables of the XAJ model (as shown in Table 1).  $x(t)$  represents the  
211 input variables of the XAJ model ( $P_{obs}$  and  $E_{obs}$ ).  $y(t)$  represents the output of the XAJ model ( $Q$ ).  
212  $\varphi_f$  and  $\varphi_g$  are parameters in the XAJ model (as shown in Table 3).  $F(\cdot)$  and  $G(\cdot)$  represent the  
213 mathematical equations and functions in the model. The above equations form explicit continuous  
214 equations, but in practice, implicit discrete equations are generally used to obtain numerical solutions:

$$215 \begin{cases} h(t) = f(h(t-1), x(t); \varphi_f) \\ y(t) = g(h(t), x(t); \varphi_g) \end{cases} \quad (2)$$

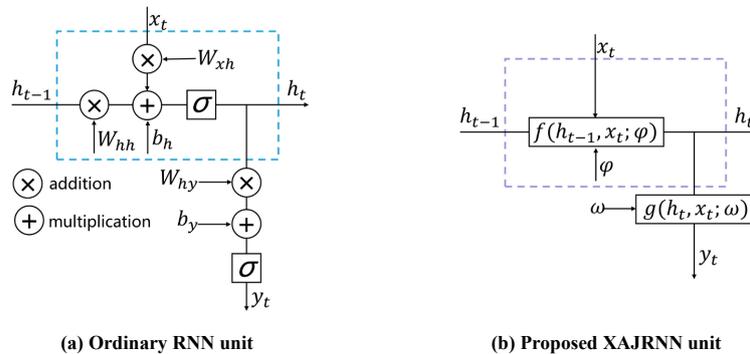
216 Ordinary RNN is neural network structures specifically designed for handling sequential data, as  
217 shown in Figure 3(a). RNN utilizes time-dependent relationships in sequences by storing previous state  
218 information to assist in current computations (Rumelhart et al., 1986). At  $t$ th time step, the calculation  
219 in an RNN unit can be divided into two steps: the first step is updating the hidden state ( $h_t$ ), and the  
220 second step is calculating the output ( $y_t$ ). The calculation formulas are as follows:

$$221 \begin{cases} h_t = \sigma(W_{xh} \cdot x_t + W_{hh} \cdot h_{t-1} + b_h) \\ y_t = \sigma(W_{hy} \cdot h_t + b_y) \end{cases} \quad (3)$$

222 where,  $h_t$ ,  $x_t$  and  $y_t$  are the state, input, and output at  $t$ th time, respectively.  $W_{xh}$ ,  $W_{hh}$  and  $W_{hy}$   
223 are the weight parameters.  $b_h$  and  $b_y$  are bias parameters.  $\sigma$  is the nonlinear activation function.



224 It can be observed that Eq. (2) and (3) have a similar structure, as they both combine ODE and  
 225 output equations. Therefore, in this study, we modify the ordinary RNN unit structure by replacing the  
 226 original equations and parameters with those derived from the XAJ model, resulting in the XAJRNN.  
 227 Similar to the ordinary RNN structure (Rumelhart et al., 1986), the backbone of the XAJRNN layer  
 228 consists of recurrent units that provide memory of past sequences. In the XAJRNN layer structure, the  
 229 connections between the recurrent units are represented by implicit discrete equations (Eq. 3), and the  
 230 parameters (i.e., weight parameters and bias parameters) in the ordinary RNN unit are replaced by the  
 231 physically meaningful parameters (as depict in Table 3) from the XAJ model. Niu et al. (2019)  
 232 demonstrated the connection between RNN network architecture and numerical methods for ODE,  
 233 theoretically supporting the use of XAJRNN for solving the dynamics of the XAJ model system. Table  
 234 A4 summarizes the pseudocode for implementing the XAJRNN layer.  
 235



236 **Figure 3: The structures of ordinary RNN unit and proposed XAJRNN unit.**

237 **3.2 Model setup**

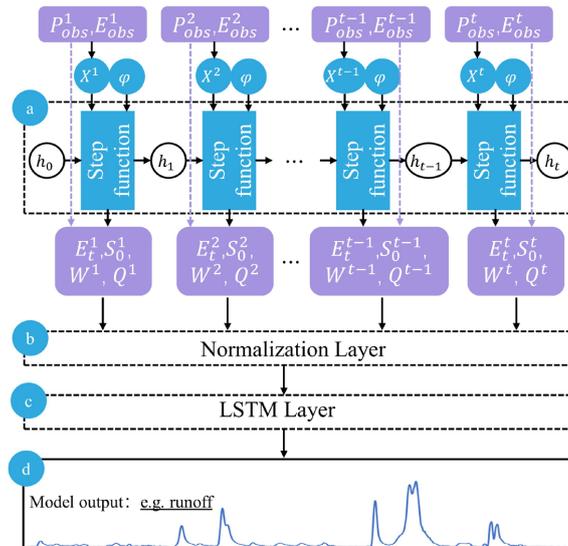
238 **3.2.1 EDL model**

239 The proposed EDL model consists of the inputs, three neural network layers, and the outputs. First,  
 240 the XAJRNN layer, as discussed in Section 3.1.2, processes the input data to generate outputs. This neural  
 241 network layer follows the water balance principle and uses the physical sub-processes of the XAJ model  
 242 to describe the runoff generation and routing process. The output variables, significantly influenced by  
 243 the runoff process, are then passed to the Normalization layer. The purpose of this layer is to normalize



244 the data, helping the EDL model converge faster during training, increasing training stability, and  
 245 reducing the impact of differences between features. Specifically, the normalization layer adjusts the data  
 246 so that the mean is 0 and the standard deviation is 1. The normalized data is then passed into the LSTM  
 247 layer for training. The choice of LSTM is based on the numerous studies demonstrating its ability to  
 248 improve the performance of hydrological model simulations. Finally, the trained EDL model outputs the  
 249 simulated runoff.

250



251

252 **Figure 4: The structure of the proposed EDL model. (a) The structure network schematic graph of the**  
 253 **XAJRNN layer.  $h$  represents the state variables in the XAJRNN layer (as shown in Table A1).  $\varphi$  represents**  
 254 **the parameters in the XAJRNN layer (as shown in Table A3). (b), (c), and (d) represent the normalization**  
 255 **layer, LSTM layer, and output results, respectively.**

256 For the EDL model, similar to the traditional XAJ model, the XAJRNN layer takes areal mean  
 257 rainfall ( $P_{obs}$ ) and pan evaporation ( $E_{obs}$ ) as input data, with a shape of [batch size, sequence length, 2  
 258 (input feature dimensions)]. The output physical quantities of interest are the actual evapotranspiration  
 259 ( $E_t$ ), the areal mean free water storage ( $S_0$ ), the areal mean tension water storage ( $W$ ), and outflow  
 260 discharge of the basin ( $Q$ ). These four physical quantities, along with the two input sequences, form a  
 261 new sequence that serves as input for subsequent layers. The shape of the new input is [batch size,  
 262 sequence length, 6 (new input feature dimensions)]. After passing through normalization layers and



263 LSTM layers, the final simulated flow sequence is obtained. The EDL model is trained using the *Adam*  
264 optimization algorithm, with *NSE* as the loss function and a learning rate of 0.001 for parameter  
265 estimation. The maximum number of iterations is set to 200, and training samples are reused in each  
266 training cycle until convergence is achieved (i.e., the absolute difference in *NSE* between consecutive  
267 cycles is less than 0.001).

### 268 3.2.1 Benchmark model

269 To compare the performance of the EDL model, two benchmark models are established. The first  
270 benchmark model is the LSTM model, which only uses the LSTM neural network layers. The input is  
271 the observed rainfall ( $P_{obs}$ ) and pan evaporation ( $E_{obs}$ ), the output is the simulated flow discharge. In order  
272 to reduce the impact of the training process on the model performance, the training process and  
273 hyperparameters of the LSTM model are the same as those of the EDL model.

274 The second benchmark model is the ordinary Xin'anjiang model, which also takes rainfall and  
275 evaporation as input to obtain the final simulated flow. Unlike the previous DL model, we use the genetic  
276 algorithm (GA) to calibrate model parameters. The GA searches in a population of points, uses the  
277 encoding of parameter sets, and uses probabilistic transition rules. There are four GA hyperparameters:  
278 crossover probability parameter ( $p_c$ ), mutation probability parameter ( $p_m$ ), population size parameter ( $p_{size}$ )  
279 and the maximum number of generation ( $T_{max}$ ). Referring to the research results of Cheng et al. (2006),  
280 the above hyperparameters are set to,  $p_c=0.8$ ,  $p_m=0.1$ ,  $p_{size}=150$ , and  $T_{max}=1500$ .

### 281 3.3 Evaluation metrics

282 The overall performance of the models is evaluated using *NSE* (Nash and Sutcliffe, 1970), relative  
283 error (*RE*), and root mean squared error (*RMSE*). The calculation formulas are as follows:

$$284 \quad NSE = 1 - \frac{\sum_{i=1}^N (Q_{o,i} - Q_{f,i})^2}{\sum_{i=1}^N (Q_{o,i} - \bar{Q}_o)^2} \quad (4)$$

$$285 \quad RE = \frac{\sum_{i=1}^N Q_{f,i} - \sum_{i=1}^N Q_{o,i}}{\sum_{i=1}^N Q_{o,i}} \times 100\% \quad (5)$$

$$286 \quad RMSE = \sqrt{\frac{\sum_{i=1}^N (Q_{f,i} - Q_{o,i})^2}{N}} \quad (6)$$

287 where  $N$  is the number of samples,  $Q_o$ ,  $\bar{Q}_o$  and  $Q_{f,i}$  represent the observed inflows, mean value,



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288 and simulated inflows, respectively.

289 To further illustrate the performance of the three models in flood simulation, the flood peak relative  
290 error (*PRE*) and the flood peak timing difference ( $\Delta T$ ) will be used to evaluate the simulating  
291 performance. The calculation formulas are as follows:

$$292 \quad PRE = \frac{Q_{f,peak} - Q_{o,peak}}{Q_{o,peak}} \times 100\% \quad (7)$$

$$293 \quad \Delta T = T_o - T_f \quad (8)$$

294 where  $Q_{o,peak}$  and  $Q_{f,peak}$  represent the observed and simulated peak inflow discharge.  $T_o$  and  $T_f$   
295 are the observed and simulated times of peak discharges occurred. If  $\Delta T$  is positive, the simulated peak  
296 discharge occurs early than the observed peak discharge; and vis versa.

## 297 4 Results

### 298 4.1 Comparison of model performance

299 Table 1 presents the evaluation metrics for flood simulation using three models – EDL, XAJ, and  
300 LSTM – across two different river basins, namely Lushui River and Qingjiang River basins. The  
301 evaluation metrics includes *NSE*, *RE*, and *RMSE* values for both training and test phases. When  
302 simulating floods in the Lushui River basin, the EDL model achieved an *NSE* of 0.98, an *RE* below 3%,  
303 and a significantly lower *RMSE* compared to benchmark models, demonstrating a clear advantage. The  
304 performance of the LSTM model was similar to that of the EDL model but slightly inferior in terms of  
305 *RMSE* and *NSE*. In contrast, the traditional XAJ model yielded lower *NSE* values, larger *RE* deviations,  
306 and the highest *RMSE* values during both training and test phases, indicating significantly poorer  
307 simulation accuracy and stability compared to the DL models.

308 When simulating floods in the Qingjiang River basin, the overall performance of the three models  
309 was not as strong as in the Lushui River basin. However, the EDL model still performed best during the  
310 training phase, achieving the highest *NSE* (0.95), the lowest *RE* (1.1%), and an *RMSE* of 104.09 m<sup>3</sup>/s.  
311 During the testing period, its performance was comparable to that of the LSTM model. In conclusion,  
312 the EDL model demonstrated exceptional flood simulation capabilities under intricate basin conditions,  
313 highlighting its substantial potential in flood simulation and forecasting.



314 **Table 1: Comparative analysis of model simulation accuracy evaluation metrics.**

Basin	Model	Training period			Test period		
		<i>NSE</i>	<i>RE</i> (%)	<i>RMSE</i> (m <sup>3</sup> /s)	<i>NSE</i>	<i>RE</i> (%)	<i>RMSE</i> (m <sup>3</sup> /s)
Lushui River	EDL	0.98	1.59	34.11	0.98	-2.69	43.71
	XAJ	0.86	-26.07	93.83	0.9	-18.5	89.6
	LSTM	0.97	-1.9	44.87	0.96	-0.61	54.27
Qingjiang River	EDL	0.95	1.1	104.09	0.92	-8.74	167.94
	XAJ	0.85	5.91	182.05	0.85	-7.92	231.17
	LSTM	0.9	-4.16	147.89	0.93	-6.19	155.71

315

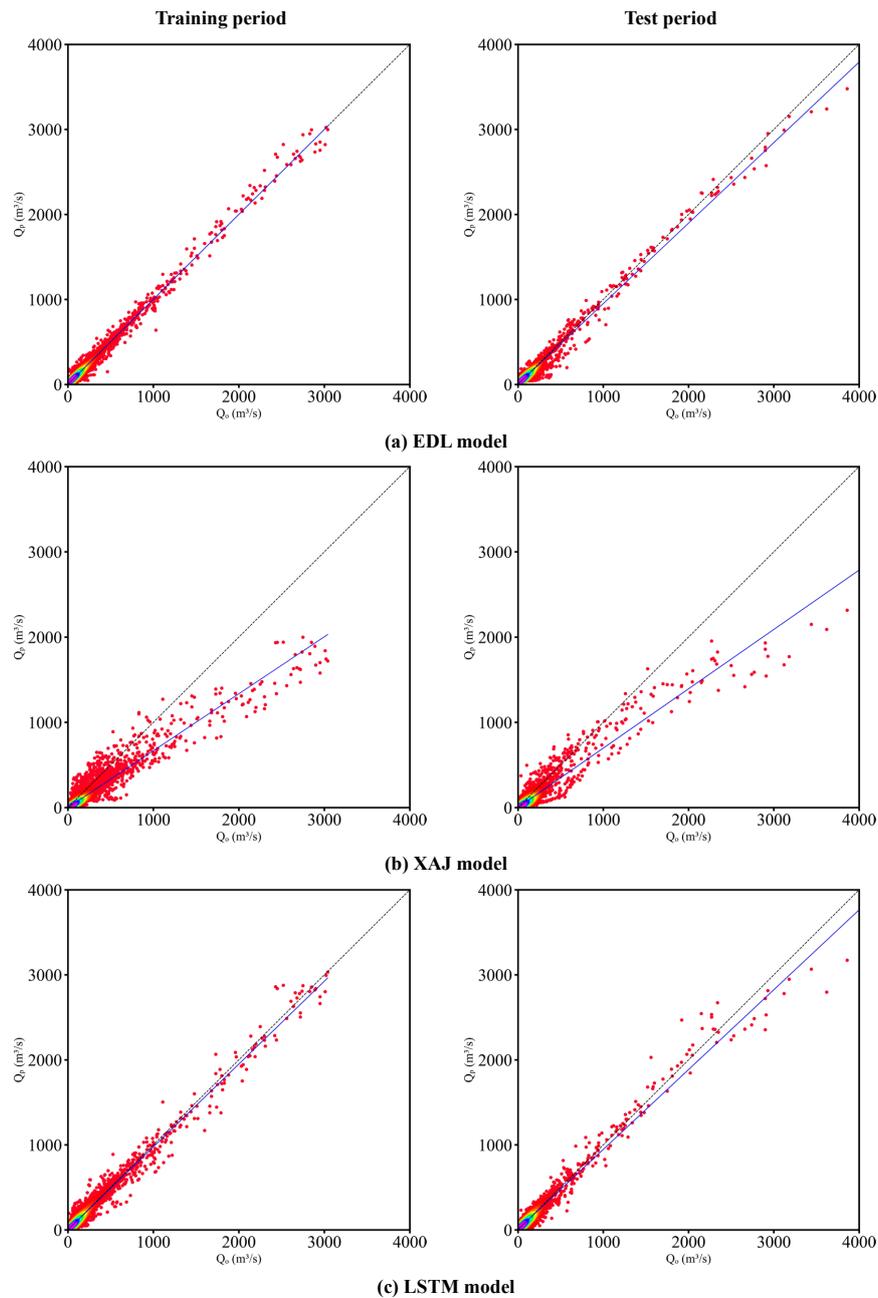
316 Figure 5 and Figure 6 respectively present the scatter plots of flood simulation results for the Lushui  
 317 River and Qingjiang River basins using the EDL model, the XAJ model, and the LSTM model. In Figure  
 318 5(a), during the training period, the scatter points of the EDL model are tightly clustered and evenly  
 319 distributed around the 1:1 ideal line. However, during the test period, in the high flow range, most of the  
 320 scatter points are located below the 1:1 ideal line. As shown in Figure 5(b), the scatter points of the XAJ  
 321 model are more dispersed in the low to medium flow range during the training period compared to the  
 322 EDL model. In the high flow range, the scatter points are significantly below the 1:1 ideal line, with a  
 323 similar distribution during the test period. In Figure 5(c), the scatter points of the LSTM model during  
 324 the training period are evenly distributed around the 1:1 ideal line but are more dispersed than those of  
 325 the EDL model. During the test period, the scatter points in the low to medium flow range are evenly  
 326 distributed around the 1:1 ideal line, similar to the EDL model, but in the high flow range, most scatter  
 327 points are below the 1:1 ideal line. Compared to the EDL model, the scatter points of the LSTM model  
 328 deviate more noticeably from the 1:1 ideal line. Therefore, it can be concluded that the scatter plots of  
 329 the EDL model are relatively better, while the scatter plots of the XAJ and LSTM models are relatively  
 330 worse.

331 In Figure 6 (a), the scatter points of the EDL model are very compact and evenly distributed on both  
 332 sides of the 1:1 ideal line during the training period. However, the scatter points are more loosely  
 333 distributed, and some scatter points are obviously below the 1:1 ideal line during the test period. As  
 334 shown in Figure 6 (b), the scatter points of the XAJ model during the training period are more scattered  
 335 than the DEL model in the low to medium flow range, and the scatter points are obviously deviated from

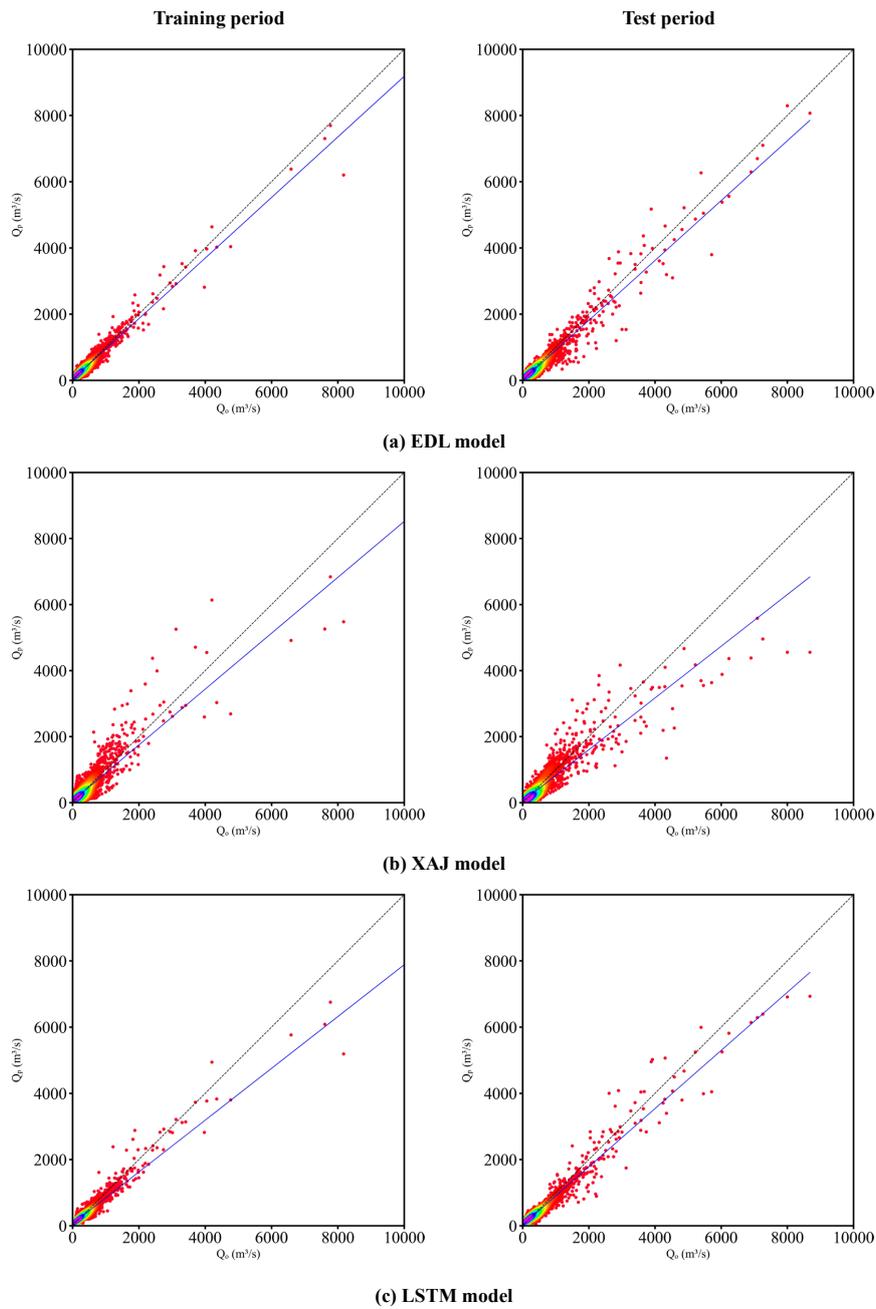


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336 the 1:1 ideal line in the high flow range. During the test period, the scatter point distribution of the XAJ  
337 model is looser, and the scatter points are farther from the 1:1 ideal line in the high flow range. As shown  
338 in Figure 6 (c), the scatter point distribution of the LSTM model during the training period is similar to  
339 that of the DEL model, but the scatter points deviate more obviously from the 1:1 ideal line in the high  
340 flow range. During the test period, it is also similar to the DEL model, but the scatter points are obviously  
341 below the 1:1 ideal line in the high flow range. Therefore, it can be concluded that the scatter plots of the  
342 DEL model are relatively better than these of the XAJ and LSTM models.  
343



344 **Figure 5: Scatter plots of observed ( $Q_o$ ) and simulated ( $Q_p$ ) flow discharges by three models in the Lushui**  
345 **River basin.**



346 **Figure 6: Scatter plots of observed ( $Q_o$ ) and simulated ( $Q_p$ ) flow discharge by three models in the Qingjiang**  
347 **River basin.**



---

#### 348 4.2 Comparison of the effectiveness of flood events simulation

349 Four major flood processes during the test period were selected in the Lushui River and Qingjiang  
350 River basins as case study. The simulation evaluation metrics of the three models (EDL model, XAJ  
351 model, and LSTM model) in these four flood processes are shown in Tables 2 and 3, respectively. These  
352 evaluation metrics include *NSE*, *RE*, *RMSE*, *PRE*, and  $\Delta T$ .

353 In the Lushui River basin, the EDL model performed exceptionally well with high simulation  
354 accuracy, the *NSE* ranged from 0.97 to 0.99, *RE* ranged from -7.54% to -1.9%, and *RMSE* was as low as  
355 71.66 m<sup>3</sup>/s. Additionally, the EDL model's *PRE* was consistently below -12%, and  $\Delta T$  remained at 0,  
356 highlighting its high reliability in simulating peak flow magnitude and timing. In contrast, the XAJ  
357 model's *NSE* ranged from 0.65 to 0.93, with significant *RE* deviations and *RMSE* values much higher  
358 than those of the EDL model, resulting in subpar overall performance. The LSTM model's *NSE* ranged  
359 from 0.91 to 0.97, close to that of the EDL model, but its *RE* and *RMSE* were slightly less favorable,  
360 resulting in marginally lower simulation accuracy.

361 In the Qingjiang River basin, the EDL model continued to demonstrate superior performance, with  
362 *NSE* exceeding 0.95 in all cases except for extreme events, *RE* ranging from -4.7% to -0.17% with  
363 minimal bias, and *RMSE* as low as 266.62 m<sup>3</sup>/s. Although the EDL model's performance slightly declined  
364 during extreme events (e.g., 20200726), it still outperformed other models overall. The XAJ model's  
365 performance in the Qingjiang River basin was significantly inferior to the EDL model, with *NSE* varying  
366 widely, reaching as low as 0.32, *RE* deviations as high as 26.42%, and *RMSE* peaking at 1277.61 m<sup>3</sup>/s,  
367 indicating its poor adaptability to complex events. The LSTM model's *NSE* ranged from 0.64 to 0.94,  
368 overall better than the XAJ model, but its accuracy and timeliness in peak flow simulation were  
369 insufficient during extreme events.

370 In summary, the EDL model exhibited the best overall performance in flood simulations for both  
371 the Lushui and Qingjiang River basins, with high accuracy, low bias, and excellent stability, particularly  
372 in regular flood events. Although the LSTM model's performance was close to that of the EDL model  
373 overall, it was slightly lacking in extreme events. In comparison, the XAJ model lagged significantly in  
374 both accuracy and adaptability, making it less suitable for precise flood simulation.



375 The outstanding performance of the EDL model highlights its immense potential in flood simulation,  
376 especially in complex basin conditions and extreme flood events. This further proves the advancement  
377 and feasibility of the model obtained by coupling deep learning technology with traditional hydrological  
378 models in the field of hydrological simulation, and provides strong tool support for solving flood  
379 forecasting problems.

380

381 **Table 2: Results of flood simulation evaluation metrics for different events in the Lushui River basin.**

Flood event	Model	<i>NSE</i>	<i>RE</i> (%)	<i>RMSE</i> (m <sup>3</sup> /s)	<i>PRE</i> (%)	$\Delta T$ (h)
20170624	EDL	0.98	-7.54	211.98	-11.99	0
	XAJ	0.83	-19.31	561.31	-26.62	0
	LSTM	0.91	-12.29	421.53	-21.7	-3
20170702	EDL	0.97	-3.53	138.01	-11.57	0
	XAJ	0.65	-24.8	468.94	-37.34	30
	LSTM	0.93	0.76	204.43	-12.59	27
20170813	EDL	0.99	-1.9	71.66	-0.9	0
	XAJ	0.85	-18.28	351.25	-26.61	3
	LSTM	0.97	0.28	142.23	-7.31	0
20190526	EDL	0.98	-3.85	85.92	-0.78	0
	XAJ	0.93	1.23	175.86	-10.15	0
	LSTM	0.97	-4.49	109.74	0.45	0

382

383



384 **Table 3: Results of flood simulation evaluation metrics for different events in the Qingjiang River basin.**

Flood event	Model	<i>NSE</i>	<i>RE</i> (%)	<i>RMSE</i> (m <sup>3</sup> /s)	<i>PRE</i> (%)	$\Delta T$ (h)
20171003	EDL	0.95	-4.43	244.26	-7.64	0
	XAJ	0.89	5.38	357.55	-8.59	0
	LSTM	0.85	-15.82	417.92	-27.02	0
20200628	EDL	0.98	-0.17	266.62	-2.2	0
	XAJ	0.95	5.48	467.13	-7.34	0
	LSTM	0.94	-3.58	506.72	-11.95	0
20200717	EDL	0.95	-1.74	533.14	-4.48	6
	XAJ	0.66	-23.15	1368.23	-28.61	0
	LSTM	0.91	-5.43	696.92	-20.18	0
20200726	EDL	0.61	-4.7	966.73	-9.45	-6
	XAJ	0.32	26.42	1277.61	-12.75	-6
	LSTM	0.64	1.84	931.87	-13.29	-6

385

386 To visually demonstrate the advantages of the EDL model, Figure 7 and 8 respectively present the  
 387 hydrographs of four flood events in the Lushui River and Qingjiang River basins, comparing the  
 388 simulation results of the EDL model, XAJRNN model, and LSTM model.

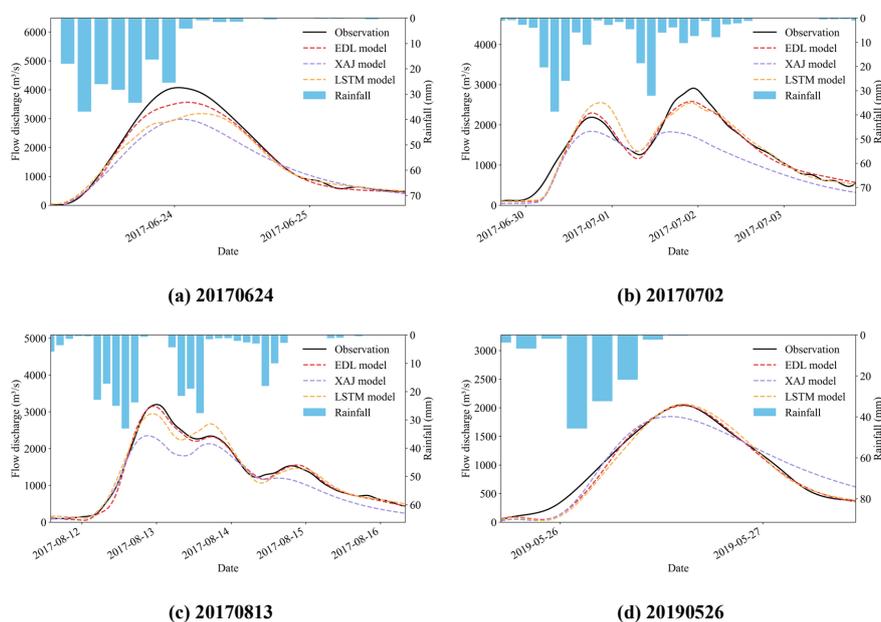
389 From Figure 7, it can be observed that the flood event in 20170624, all three models underestimated  
 390 the peak flow to varying degrees, but the DEL model performed relatively better and more accurately  
 391 simulated the timing of the peak flow. In the 20170702 and 20170813 compound flood events, the DEL  
 392 model's simulated hydrograph during the peak flow phase was closer to the observed hydrograph  
 393 compared to the XAJ model and the LSTM model. During flood event in 20190526, both the DEL model  
 394 and the LSTM model simulated the peak flow phase well. However, in the 20170702 and 20190526 flood  
 395 events, all three models exhibited delays, as evidenced by discrepancies in the rising speed during the  
 396 flood rising phase compared to the observations. This may be related to the models' insufficient ability  
 397 to simulate low flow conditions. Overall, the DEL model performed well in simulating the hydrographs  
 398 of the Lushui River basin, accurately capturing both the peak flow and the timing of the peak.

399 Compared to the Lushui River basin, the simulation results of the three models in the Qingjiang  
 400 River basin showed certain limitations, which were particularly evident in the 20200726 flood event as  
 401 shown in Figure 8. All three models underestimated the peak flow, and the simulated peak was  
 402 significantly delayed compared to the observed peak, indicating potential errors in the models' calculation

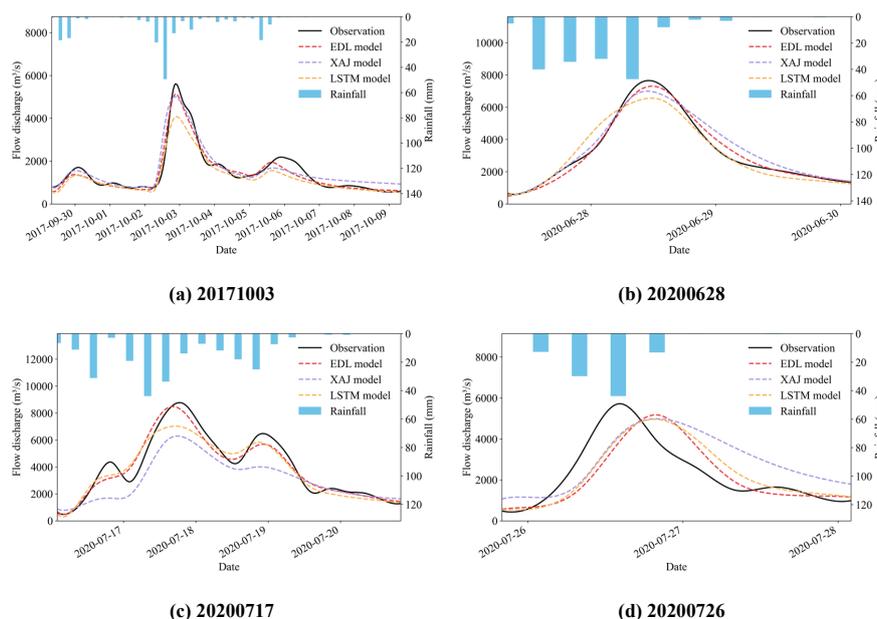


403 of the flow routing process, especially under complex terrain conditions. For the 20201003 and 20200717  
404 flood events, the DEL model's simulated hydrograph was closer to the observed hydrograph compared  
405 to the XAJ model and the LSTM model. For flood event in 20200628, the LSTM model performed better  
406 during the recession phase but significantly underestimated the peak flow and failed to accurately  
407 simulate the rising phase. In contrast, the DEL model performed better during the rising and peak phases  
408 but exhibited delays during the recession phase. Overall, although some deviations in peak flow and  
409 timing exist, the DEL model still effectively captures the general flood trends in the Qingjiang River  
410 basin.

411



412 **Figure 7: Comparison of observed and simulated flood hydrographs in the Lushui River basin.**



413 **Figure 8: Comparison of observed and simulated flood hydrographs in the Qingjiang River basin.**

414 **5 Discussion**

415 The XAJ model is a well-established hydrological model utilized for generalizing hydrological  
416 processes in a basin, including runoff generation and routing. However, when used in isolation, the model  
417 may struggle to adequately capture intricate nonlinear relationships, particularly evident in flood peak  
418 simulating where it might not fully account for the impacts of real-time meteorological changes. On the  
419 other hand, DL models, especially time-series models like LSTM, are adept at capturing complex  
420 nonlinear relationships within time series data. Nevertheless, they may encounter delays in accurately  
421 simulating flood peak timings (Chen et al., 2022; Cui et al., 2021; Xiang et al., 2024). To address this  
422 limitation, a fusion of the XAJ model and DL models can mitigate the weaknesses inherent in each  
423 approach. Specifically, the conventional hydrological model offers a foundation for physical processes  
424 that enhance the simulation of watershed hydrological responses, while the DL model can refine the  
425 output of the hydrological model, particularly in terms of temporal accuracy and the comprehension of  
426 nonlinear relationships. This hybrid approach allows the XAJ model to capture long-term dependencies  
427 in hydrological processes while enabling the DL model to make more precise simulations regarding flood



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428 peak timing, thus effectively minimizing delays in flood peak simulation.

429 In traditional processes, DL models such as LSTM are commonly employed as post-processors to  
430 rectify the outcomes of hydrological models (Cho and Kim, 2022; Cui et al., 2021; Frame et al., 2021;  
431 Han and Morrison, 2022). Nevertheless, a significant drawback of this methodology stems from the  
432 inconsistent parameter tuning. Typically, the parameters of the hydrological model are initially fine-tuned  
433 to achieve the best simulation results, followed by the utilization of an LSTM model for refinement.  
434 However, as the parameter adjustments for the hydrological and DL models are carried out independently,  
435 this lack of synchronization in tuning may result in a less-than-optimal parameter combination,  
436 subsequently impacting the accuracy of the final simulations. In contrast, the EDL model we have  
437 devised undergoes synchronized training within the DL framework, where all parameters are collectively  
438 optimized. This strategy ensures that the parameters of the hydrological and DL models are  
439 simultaneously fine-tuned during training, leading to the optimal parameter combination and enhancing  
440 simulation accuracy. By tackling the inherent parameter mismatch issue seen in conventional approaches,  
441 this methodology elevates the overall performance of the model.

## 442 **6 Conclusion**

443 The present study proposes a novel EDL model that combines the physics-driven XAJRNN layer  
444 with the LSTM layer, successfully achieving accurate simulation of flood processes in the Lushui River  
445 basin and Qingjiang River basin. This model leverages the physical mechanisms of the XAJ model and  
446 the nonlinear representation capabilities of DL, demonstrating strong simulation performance. The key  
447 findings of this study are as summarized as follows:

448 (1) The EDL model demonstrates superior performance in both simulation accuracy and error  
449 control. It achieves an average *NSE* of 0.98 in the Lushui River basin and 0.94 in the Qingjiang River  
450 basin, demonstrating its outstanding fitting capability. Its average *RMSE* is 38.91 m<sup>3</sup>/s in the Lushui River  
451 basin and 136.02 m<sup>3</sup>/s in the Qingjiang River basin, significantly lower than that of benchmark models,  
452 highlighting its superior simulation accuracy. Although the *RE* is slightly higher during the testing phase,  
453 the combined analysis of the training phase *RE* shows that the EDL model consistently outperforms its



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454 counterparts with stable error control.

455 (2) The EDL model demonstrates the highest stability in most flood simulations. Compared to the  
456 XAJ and LSTM models, the EDL model achieves smaller *PRE* values, indicating its superior accuracy  
457 in simulating flood peak magnitudes. Moreover, except for a few rare cases, the EDL model's  $\Delta T$  is nearly  
458 zero, showcasing its unparalleled precision in simulating the timing of flood peaks.

459 (3) Compared to traditional single models, the EDL model not only significantly improves  
460 simulation accuracy but also enhances interpretability by integrating physical mechanisms. This  
461 innovative approach paves the way for the seamless integration of deep learning with hydrological  
462 physical mechanisms, advancing research in the field.

463 This study demonstrates that the proposed EDL model that combine physical mechanisms with DL  
464 is an effective way to improve flood simulation and forecasting accuracy. Future research should further  
465 explore how to more closely integrate complex physical mechanisms with neural network models to  
466 achieve higher simulative capabilities and scientific discovery potential.

#### 467 **Code availability**

468 The code used to support the findings of this study are available from the corresponding author upon  
469 request.

#### 470 **Data availability**

471 The data generated and/or analyzed during the current study are not publicly available for legal/ethical  
472 reasons but are available from the corresponding author on reasonable request.

#### 473 **Author contributions**

474 Xin Xiang and Shenglian Guo conceived and designed the experiments; Xin Xiang performed the  
475 experiments and wrote the manuscript draft; Xin Xiang, Shenglian Guo, Chenglong Li, and Yun Wang  
476 reviewed and edited the manuscript.



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477 **Competing interests**

478 The authors declare that they have no conflict of interest.

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482 suggestions help to improve the manuscript.




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483 **Appendix A. Supplementary tables and texts**

484 Table A1 describes the state variables of the XAJ model.

485 Table A2 describes the flux of the XAJ model.

486 Table A3 describes parameters and their value ranges of the XAJ model.

487 Table A4 describes the pseudocode of the XAJRNN layer.

488 Text A1 describes the details of the XAJ model.

489 **Table A1: State variables of the XAJ model.**

Module	State variable	Meaning	Unit
Evapotranspiration	$W_u$	Areal mean tension water storage of the upper soil layer	mm
	$W_l$	Areal mean tension water storage of the lower soil layer	
	$W_d$	Areal mean tension water storage of the deep soil layer	
Runoff separation	$S_0$	Areal mean free water storage	
Flow routing	$O_i$	Water storage of the interflow linear reservoir	
	$O_g$	Water storage of the groundwater linear reservoir	
	$F_1$	Water storage of the first reservoir in the Nash unit hydrograph	
	$F_2$	Water storage of the second reservoir in the Nash unit hydrograph	
	$F_3$	Water storage of the third reservoir in the Nash unit hydrograph	

490



491 **Table A2: Flux of the XAJ model.**

Module	Flux	Meaning	Unit
Evapotranspiration	$P_{obs}$	Areal mean rainfall	$mm/\Delta t$
	$E_{obs}$	Measured pan evaporation	
	$P$	Areal mean rainfall of the impervious area	
	$R_{imp}$	Runoff directly from the impervious area	
	$P_n$	Areal mean net rainfall	
	$E_p$	Potential evapotranspiration	
	$E_u$	Actual evapotranspiration of the upper soil layer	
	$E_l$	Actual evapotranspiration of the lower soil layer	
	$E_d$	Actual evapotranspiration of the deep soil layer	
Runoff generation	$E_t$	Actual evapotranspiration	$mm/\Delta t$
	$R$	Runoff produced from the previous area	
Runoff separation	$R_s$	Surface runoff	$mm/\Delta t$
	$R_i$	Interflow runoff	
	$R_g$	Groundwater runoff	
Flow routing	$Q_i$	Outflow of the interflow linear reservoir	$mm/\Delta t$
	$Q_g$	Outflow of the groundwater linear reservoir	
	$Q_t$	Total inflow to channel network	
	$Q_1$	Outflow of the first reservoir in the Nash unit hydrograph	
	$Q_2$	Outflow of the second reservoir in the Nash unit hydrograph	
	$Q_3$	Outflow of the third reservoir in the Nash unit hydrograph	
	$Q$	Outflow discharge of the basin	

492



493 **Table A3: Parameters and their value ranges of the XAJ model.**

Module	Parameter	Meaning	Value range	Unit
Evapotranspiration	$K_c$	Ratio of potential evapotranspiration to pan evapotranspiration	[0.6,1.5]	-
	$c$	Coefficient of deep evapotranspiration	[0.01,0.2]	-
	$W_{um}$	Areal mean tension water capacity of the upper soil layer	[5,30]	mm
	$W_{lm}$	Areal mean tension water capacity of the lower soil layer	[60,90]	mm
	$W_{dm}$	Areal mean tension water capacity of the deep soil layer	[15,60]	mm
	$A_{imp}$	Ratio of the impervious area	[0.01,0.2]	-
Runoff generation	$b$	Exponent of the tension water capacity curve	[0.1,0.4]	-
Runoff separation	$S_m$	Areal mean of the free water capacity of the surface soil layer	[10,50]	mm
	$ex$	Exponent of the free water capacity curve	[1,1.5]	-
	$K_i$	Outflow coefficient of the free water storage to interflow	[0.1,0.55]	-
	$K_g$	Outflow coefficient of the free water storage to groundwater	[0.7- $K_i$ ]	-
Flow routing	$c_i$	Recession constant of interflow storage	[0.1,0.9]	-
	$c_g$	Recession constant of groundwater storage	[0.9,0.988]	-
	$K_f$	Storage-discharge coefficient of the linear reservoir in the Nash unit hydrograph	[0.1,10]	-

494



495 **Table A4: Pseudocode of the XAJRNN layer.**

**Algorithm:** the XAJRNN layer

**Input:** Sequences of observed rainfall  $\{P_{obs}\}$  and observed evapotranspiration  $\{E_{obs}\}$

**State initialization:**  $W_u^{(0)} = 0, W_l^{(0)} = 0, W_d^{(0)} = 0, S_0^{(0)} = 0, O_i^{(0)} = 0, O_g^{(0)} = 0, O_s^{(0)} = 0, F_1^{(0)} = 0, F_2^{(0)} = 0$  and  $F_3^{(0)} = 0$

**Parameters:**  $K_c, c, W_{um}, W_{lm}, W_{dm}, A_{imp}, b, S_m, ex, K_i, K_g, c_i, c_g, K_f, n$

**function** step\_function ( $[P^{(i)}, E^{(i)}], [W_u^{(i-1)}, W_l^{(i-1)}, W_d^{(i-1)}, S_0^{(i-1)}, O_i^{(i-1)}, O_g^{(i-1)}, O_s^{(i-1)}, F_1^{(i-1)}, F_2^{(i-1)}, F_3^{(i-1)}],$  parameters):

Calculate  $R^{(i)}, R_{imp}^{(i)}, E_t^{(i)}, P_n^{(i)}, W_u^{(i)}, W_l^{(i)}, W_d^{(i)}$  via Eqs. (A1) – (A20)

Calculate  $R_s^{(i)}, R_i^{(i)}, R_g^{(i)}, S_0^{(i)}$  via Eqs. (A21) – (A26)

Calculate  $Q_i^{(i)}, Q_g^{(i)}, Q_t^{(i)}, O_i^{(i)}, O_g^{(i)}$  via Eqs. (A27) – (A29)

Calculate  $Q_1^{(i)}, Q_2^{(i)}, Q_3^{(i)}, F_1^{(i)}, F_2^{(i)}, F_3^{(i)}$  via Eqs. (A30) – (A32)

**return**  $W_u^{(i)}, W_l^{(i)}, W_d^{(i)}, S_0^{(i)}, O_i^{(i)}, O_g^{(i)}, O_s^{(i)}, F_1^{(i)}, F_2^{(i)}$  and  $F_3^{(i)}$

**do** RNN (step function,  $[\{P\}, \{E\}], [W_u^{(0)}, W_l^{(0)}, W_d^{(0)}, S_0^{(0)}, O_i^{(0)}, O_g^{(0)}, O_s^{(0)}, F_1^{(0)}, F_2^{(0)}, F_3^{(0)}]$ )  
 to obtain sequences of  $\{W_u\}, \{W_l\}, \{W_d\}, \{S_0\}, \{O_i\}, \{O_g\}, \{O_s\}, \{F_1\}, \{F_2\}, \{F_3\}$

Calculate sequence of  $\{Q\}$  via Eq. (A33)

**Output:** The sequence of runoff at the catchment outlet  $\{Q\}$

496



497 **Text A1**

498 In the evapotranspiration, considering the uneven vertical distribution of soil, the XAJ model  
 499 divides the soil into three layers and calculates the actual evapotranspiration using a three-layer soil  
 500 moisture model. The calculation principle is as follows: The upper layer evaporates according to its  
 501 evapotranspiration capacity. When the upper layer's water content is insufficient, the remaining  
 502 evapotranspiration capacity is supplied by evaporation from the lower layers. The evaporation from the  
 503 lower layers is proportional to the water storage in those layers. The ratio of the evaporation from the  
 504 lower layer to the remaining evapotranspiration capacity must not be less than the coefficient of deep  
 505 evapotranspiration ( $c$ ). Otherwise, the lower layer water storage will supply the insufficient portion. If  
 506 the lower layer water storage is not sufficient to compensate, the deep layer water storage will provide  
 507 the remainder. The calculation formula is as follows:

$$508 \quad P = P_{obs}(1 - A_{imp}) \quad (A1)$$

$$509 \quad R_{imp} = P_{obs} \times A_{imp}$$

$$510 \quad E_p = K_c E_{obs} \quad (A2)$$

511 (1) When  $W_u + P \geq E_p$ ,

$$512 \quad E_u = E_p; E_l = 0; E_d = 0 \quad (A2)$$

513 (2) When  $W_u + P < E_p$  and  $W_l \geq c \times W_{lm}$ ,

$$514 \quad E_u = W_u + P; E_l = (E_p - E_u) \times W_l / W_{lm}; E_d = 0 \quad (A3)$$

515 (3) When  $W_u + P < E_p$  and  $c \times (E_p - E_u) \leq W_l < c \times W_{lm}$ ,

$$516 \quad E_u = W_u + P; E_l = c \times (E_p - E_u); E_d = 0 \quad (A4)$$

517 (4) When  $W_u + P < E_p$  and  $c \times (E_p - E_u) > W_l$ ,

$$518 \quad E_u = W_u + P; E_l = W_l; E_d = c \times (E_p - E_u) - E_l \quad (A5)$$

$$519 \quad E_t = E_u + E_l + E_d \quad (A6)$$

$$520 \quad P_n = \begin{cases} P - E_t, & P \geq E_t \\ 0, & P < E_t \end{cases} \quad (A7)$$

521 The runoff generation calculation uses the tension water capacity curve. First, it is necessary to  
 522 calculate the areal mean tension water storage ( $W$ ) and the areal mean tension water capacity ( $W_m$ ):

$$523 \quad W = W_u + W_l + W_d \quad (A8)$$

$$524 \quad W_m = W_{um} + W_{lm} + W_{dm} \quad (A9)$$



525 The vertical coordinate value ( $\alpha$ ) corresponding to the areal mean tension water storage ( $W$ ) on the  
 526 tension water capacity curve is calculated as:

$$527 \quad \alpha = W_m \times (b + 1) \times \left[ 1 - \left( 1 - \frac{W}{W_m} \right)^{\frac{1}{1+b}} \right] \quad (\text{A11})$$

528 Calculate the runoff produced from the previous area:

$$529 \quad R = \begin{cases} P_n + W - W_m + W_m \left( 1 - \frac{P_n + \alpha}{W_m \times (b+1)} \right)^{b+1}, & P_n + \alpha \leq W_m \times (b + 1) \\ P_n + W - W_m, & P_n + \alpha > W_m \times (b + 1) \end{cases} \quad (\text{A12})$$

530 Finally, update the areal mean tension water storage of the upper, lower, and deep soil layer of the  
 531 watershed at the end of the current period, which will serve as the initial values for the next period:

$$532 \quad W_u = W_u + P - E_t - R \quad (\text{A13})$$

$$533 \quad W_l = W_l - E_l \quad (\text{A14})$$

$$534 \quad W_d = \max(W_d - E_d, 0) \quad (\text{A15})$$

535 When  $W_u > W_{um}$ ,

$$536 \quad W_l = W_l + W_u - W_{um} \quad (\text{A16})$$

$$537 \quad W_u = W_{um} \quad (\text{A17})$$

538 When  $W_l > W_{lm}$ ,

$$539 \quad W_d = W_d + W_l - W_{lm} \quad (\text{A18})$$

$$540 \quad W_l = W_{lm} \quad (\text{A19})$$

$$541 \quad W_d = \min(W_d, W_{dm}) \quad (\text{A20})$$

542 The runoff separation uses the free water capacity curve. The vertical coordinate value ( $\beta$ )  
 543 corresponding to the areal mean free water storage ( $S_0$ ) is:

$$544 \quad \beta = S_m \times (ex + 1) \times \left[ 1 - \left( 1 - S_0/S_m \right)^{\frac{1}{1+ex}} \right] \quad (\text{A21})$$

545 Therefore, the surface runoff ( $R_s$ ) is:

$$546 \quad R_s = \begin{cases} R + \{S_0 - S_m + S_m [1 - \frac{(P_n + \beta)}{S_m \times (ex+1)}]^{ex+1}\} \frac{R}{P_n}, & P_n + \beta \leq S_m \times (ex + 1) \\ R + (S_0 - S_m) \frac{R}{P_n}, & P_n + \beta > S_m \times (ex + 1) \end{cases} \quad (\text{A22})$$

$$547 \quad R_s = R_s + R_{imp} \quad (\text{A23})$$

548 The interflow runoff ( $R_i$ ):

$$549 \quad R_i = K_i \times S_0 \times \frac{R}{P_n} \quad (\text{A24})$$

550 The groundwater runoff ( $R_g$ ):



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$$551 \quad R_g = K_g \times S_0 \times \frac{R}{P_n} \quad (A25)$$

552 Calculate the areal mean free water storage ( $S_0$ ) at the end of the current period, which will serve as  
553 the initial value for the next period, as:

$$554 \quad S_0 = S_0 + (R - R_s - R_i - R_g) \times \frac{P_n}{R} \quad (A26)$$

555 The flow routing module consists of two submodules: hillslope and channel network routing. The  
556 hillslope routing adopts a linear reservoir approach, while the channel network routing uses the Nash unit  
557 hydrograph. The calculation formula for the linear reservoir is as follows:

$$558 \quad Q_i = -O_i \times \ln c_i \quad (A27)$$

$$559 \quad Q_g = -O_g \times \ln c_g \quad (A28)$$

560 The total inflow to channel network is equal to the sum of the surface runoff ( $R_s$ ), the outflow of  
561 the interflow linear reservoir ( $Q_i$ ), and the outflow of the groundwater linear reservoir ( $Q_g$ ). The  
562 calculation formula is as follows:

$$563 \quad Q_t = R_s + Q_i + Q_g \quad (A29)$$

564 The calculation formula for the Nash unit hydrograph reservoir is as follows:

$$565 \quad Q_1 = F_1/K_f \quad (A30)$$

$$566 \quad Q_2 = F_2/K_f \quad (A31)$$

$$567 \quad Q_3 = F_3/K_f \quad (A32)$$

568 The calculation formula for the outflow discharge of the basin ( $Q$ ) is as follows:

$$569 \quad Q = Q_3 \times 1000 \times F/\Delta t \quad (A33)$$

570 where  $F$  is the watershed area,  $\text{km}^2$ .  $\Delta t$  is the input time step,  $s$ .



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