RUNOFF ESTIMATION BASED ON HYBRID-PHYSICS-DATA MODEL

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KEY WORDS: Runoff Estimation, Peak Runoff, HIMS, LSTM, HPD.

ABSTRACT:

Runoff estimations play an important role in water resource planning and management. Existing hydrological models can be divided into physical models and data-driven models. Although the physical model contains certain physical knowledge and can be well generalized to new scenarios, the application of physical models is limited by the high professional knowledge requirements, difficulty in obtaining data and high computational costs. The data-driven model can fit the observed data well, but the estimation may not be physically consistent. In this letter, we propose a hybrid physical data (HPD) model combining physical model and deep learning model for runoff estimation. The model uses the output of a physical hydrological model together with the driving factors as another input of the neural network to estimate the monthly runoff of the upper Heihe River Basin in China. We show that the use of the HPD model improves the quality of runoff estimation, and results in high R^2, NSE values of 0.969, and a low RMSE value of 9.645. It is indicated that the new model had an excellent learning capability to simulate runoff and flexible ability to extract complex relevant information; At the same time, the estimation capacity of peak runoff is optimized.

1. INTRODUCTION

Runoff simulation has always been one of the key research in the field of hydrology, which provides important support for the utilization of water resources, such as environmental protection, flood disaster prevention, drought monitoring, and so on(Wang et al., 2009; Kang et al., 2017; Guo et al., 2018; Gao et al., 2019). The conventional runoff simulation hydrological model estimates streamflow based on hydrophysical processes(Kang et al., 2020). These sub-processes are driven in nonlinear ways by physical mechanisms, including evapotranspiration, interception, infiltration, soil water, and groundwater exchange, as well as the influence of water conservancy projects and other human activities(Sophocleous, 2002). Hydrological models have a wide range of uses. For example,karst tunnel hydrological model (KTHM) is used for runoff simulation in karst basins with only a small amount of hydrogeological data(Li et al., 2021). Hydrologic Simulation Program-FORTRAN (HSPF) is established to simulate the hydrological processin China's Sanya River Basin(Gui et al., 2021). And HIMS model is used to solve the process simulation in an inland river basin in China, Heihe River basin(Wang et al., 2018). However, the complexity of the physical process of the hydrological model makes it difficult for people to simulate a more reasonable physical process through limited input and obtain the ideal output.

With the increasing enrichment of hydrological data and observation data and the development of artificial intelligence (AI), especially the latest development of deep learning (DL), data-driven model evolved into a budding tool for runoff simulation predictions independent of physical principles(Shen, 2018; Tikhamarine et al., 2020). Compared with the hydrological physical model containing complex hydrological processes, the data-driven model establishes the direct relationship between hydrological variables by extracting relevant information from the input data, without considering the physical mechanism of hydrological processes(Young et al., 2017; Liu et al., 2021). For example, artificial neural networks (ANNs) have been widely used in runoff estimation because of their remarkable ability to deal with highly nonlinear problems(Hsu et al., 1995; Rezaeianzadeh et al., 2014; Kratzert et al., 2018). The long short-term memory (LSTM) network, a variant of recurrent neural network (RNN), has been proved to have great potential in hydrological modeling because of its excellent time series processing ability. For example, the effective integration of meteorological observations using LSTM models helps to improve runoff prediction(Shen, 2018). Compared with existing hydrological models, LSTM architecture shows good performance in simulating rainfall-runoff in a large number of complex catchments(Kratzert, Klotz et al., 2018). The researchers also focused on the improvement of the standard LSTM architecture and proposed a network combining LSTM and fully connected layer (FC) to process the characteristics of long duration time series with different time-series information(Zhang et al., 2020).

Although the accuracy of runoff estimation using the deep learning model is improved compared with the traditional physical model, the lack of a physical mechanism becomes a major limitation of deep learning(Ebert-Uphoff et al., 2019). The deep learning model can fit the observed data well, but the estimation may not be physically consistent, which is not helpful for the discovery of physical theory(Liu et al., 2017). Moreover, neural network training is a delicate stage, which needs to adjust multiple parameters, which also greatly affects the robustness of the approach(Verrelst et al., 2012). The combination of physical models and deep learning models is a possible solution to the current problem(Willard et al., 2020). At present, there are many feasible means, such as using machine learning to build a surrogate model(Mo et al., 2019) or to correct the mismatch between simulation values of physical models and observed values(Solomatine et al., 2009), or using

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synthetic samples containing physical mechanisms for physical guidance during training, to effectively improve the simulation of flood peaks and reduce the number of negative streamflow, and strong monotonicity is still maintained even if there is a slight disturbance in the training dataset(Xie et al., 2021).

In this letter, we establish a hybrid physical data model to preliminarily combine the physical model with the depth learning model to further improve the accuracy of runoff estimation. Specifically, the output of a physically hydrological model is used as another input in the neural network model along with the drivers. Karpatne et al. showed that the prediction can be improved by using the output of the physics-based model as a feature in the ML model and the input used to drive the physics-based model for lake temperature modeling(Karpatne et al., 2017). In this experiment, the distributed hydrologic model HIMS provides a preliminary runoff estimation, which is fed into an LSTM neural network together with the driving factors to estimate the final runoff. Through the established Hybrid-Physics-Data Model, higher precision runoff estimation is successfully obtained.

The rest of this letter is organized as follows. Section 2 of this letter describes the study area and the data used in this study. The method of the data-driven model based on the physical mechanism is described in Section 3, followed by the results of section 4 and discussion in Section 5. Finally, a conclusion is drawn in part 6.

2. STUDY AREA AND DATA

The study area is in the upper Heihe River Basin. The Heihe River Basin is located in the middle of the Hexi Corridor in Northwest China and originates in the upper Heihe River Basin situated in the Qilian Mountains. The upper Heihe River Basin covers 2088.3 km^2 and ranges in elevation from 1669 m to 5247 m. The annual average temperature is between -5 and 4 °C. The annual average rainfall is between 50 and 70 m^3/s. There are few meteorological and hydrological stations in the upper Heihe River Basin, as shown in Figure 1. The Yingluoxia station is on the upstream exit of the Heihe River Basin, which controls mountainous watershed runoff.

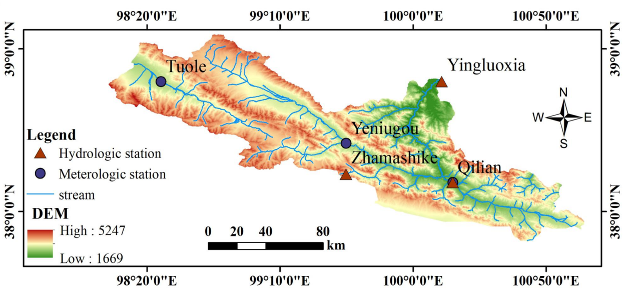

Figure 1. Upper reaches of the Heihe River Basin.

The meteorological data are from the meteorological center of the China Meteorological Administration. It includes the minimum temperature (Tmin), maximum temperature (Tmax) and precipitation (P) data of three meteorological stations in the upper Heihe River Basin, i.e. Tuole, Qilian and Yeniugou. The series is from 2000 to 2016.

Hydrological runoff data are from the Heihe River Basin Authority. It is the runoff observation data(Q) of Yingluoxia station, and the series is from 2000 to 2016.

3. METHODS

3.1 HIMS

To promote water resources management and water environment protection and provide a scientific basis for water resources management in China, a multi-scale hydrological model system was developed and named as Hydro-Informatic Modelling System (HIMS)(Liu et al., 2008). HIMS is a modular-based open framework, which can customize modules and assemble them rapidly according to the application requirements of different temporal and spatial scales.

The infiltration calculation is an empirical model, and the infiltration amount is related to rainfall, soil and vegetation:

$$f = R \cdot P^r, \tag{1}$$

Where f is infiltration capacity, P is rainfall, and parameter R and r values are parameters related to land use and soil moisture. The water balance formula for surface flow is as follows, where surface flow equals the difference between precipitation and infiltration:

$$Q_d = P - f = P - R \cdot P^r, \tag{2}$$

where Q_d is surface flow, f is infiltration capacity, and P is rainfall.

3.2 LSTM

The LSTM neural network is an improved RNN model, which was first proposed by Hochreiter and schmidhuber(Hochreiter et al., 1997). The proposal of LSTM solves the problems of gradient explosion and disappearance in RNN, and the LSTM network can also deal with complex and long-lag tasks that traditional RNNs cannot deal with. Compared with traditional RNN, LSTM introduces the concept of three gates, in which whether the input gate control allows writing, whether the forgetting gate control must update the value of the storage unit, whether the output gate control allows output. The opening or closing of the three gates is determined by the training of the dataset. The specific steps are as follows:

First, decide what information we will discard from the cellular state. This decision is made by a sigmoid layer called the "forget gate layer", which selectively forgets unnecessary information by looking at the output h_{t-1} of the previous state and the input x_t of this state.

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f), \tag{3}$$

Then decide what new information we will store in the cell state. There are two steps here. In the first step, a sigmoid layer called the "input gate layer" decides which values we'll update. Next, a tanh layer creates a vector, $\widetilde{C}_t$,containing new candidate values, which can be added to the state.

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i), \tag{4}$$

$$\widetilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] + b_C), \tag{5}$$

The second step is to update the new cell state. Update the old cell state into the new cell state.

$$C_t = f_t * C_{t-1} + i_t * \widetilde{C}_t, \tag{6}$$

Finally, we need to decide what to output. We use a sigmoid layer and a tanh layer to determine what we want to output.

$$o_t = \sigma(W_o[h_{t-1}, x_t] + b_o), \tag{7}$$

$$h_t = o_t * \tanh(C_t), \tag{8}$$

3.3 Architecture of HPD

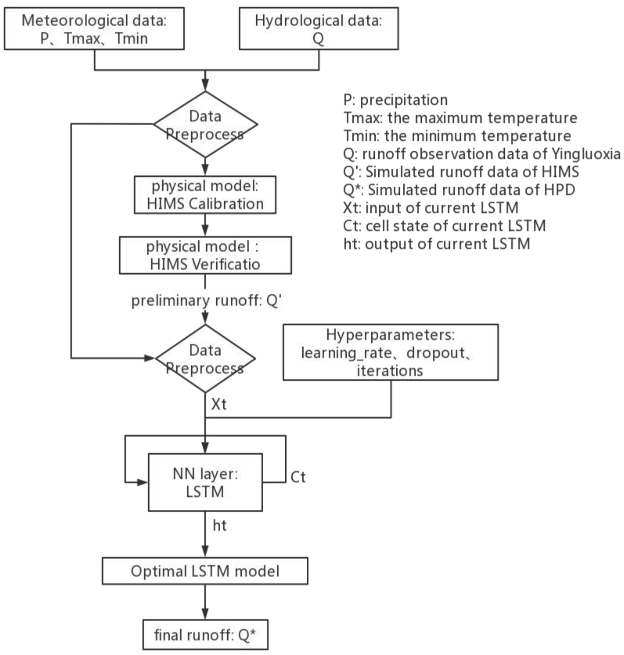

Figure 2. A schematic illustration of a hybrid-physics-data (HPD) model.

A hybrid physical data model is constructed, as shown in Figure 2. Firstly, obtain the meteorological data, precipitation data (P), maximum temperature (Tmax), minimum temperature (Tmin) and hydrological data Q in the study area from 2000 to 2016, and adjust them to the format that HIMS can read; Then, the period from 2000 to 2009 is selected as the periodic rate, and the measured data in this period are used to calibrate the HIMS model; Select 2010-2016 as the verification period to verify the calibrated HIMS; The validated HIMS model is used to estimate the runoff to obtain the preliminary runoff estimation Q' of HIMS.
Normalize the preliminary runoff estimation Q' and meteorological data P, Tmax, Tmin and hydrological data Q in the study area, and obtain monthly scale data; Taking P, Tmax, Tmin and preliminary runoff estimation Q' of multiple stations as input and runoff data as output, LSTM neural network model is constructed; The data set of time series from 2000 to 2012 was taken as the training set, and the data set of time series from 2013 to 2016 was taken as the validation set; Input learning_rate, Dropout, and iterations into the LSTM model and start training; The trained optimal LSTM model is used to obtain the final runoff Q*, and the model is evaluated.
Furthermore, HIMS may provide an incomplete representation of the target variable due to simplified or missing physics in the physical model, thus resulting in model discrepancies with respect to observations. Hence, the basic goal of HPD modeling is to combine the HIMS and LSTM to overcome their complementary deficiencies and leverage information in both physics and data. The complex features are extracted from the deep learning model to learn and make up for the systematic differences in the hydrological model.

3.4 Evaluation of Model Performance

In this letter, the data from 2000 to 2012 are used for training, and the data from 2013 to 2016 are used for verification. At the same time, root mean square error (RMSE), the coefficient of determination(R^2) and the Nash-Sutcliffe model efficiency (NSE) are used as the evaluation indicators of the accuracy of model simulation. RMSE refers to the deviation of the analogue value from the actual value. The smaller the RMSE value is, the better the estimation process is. The mathematical formula is shown below:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{N}}, \tag{9}$$

R^2 describes the degree to which the model interprets the actual value. R^2 values range with in the interval of 0 to 1. The closer the result is to 1, the better the model fitting effect. The mathematical formula is shown below:

$$R^2 = \frac{\sum_{i=1}^{N}[(y_i - \bar{y}_i)(y_i - \hat{y}_i)]^2}{\sum_{i=1}^{N}(y_i - \bar{y}_i)^2 \sum_{i=1}^{N}(\hat{y}_i - \bar{y}_i)^2}, \tag{10}$$

NSE is generally used to verify the quality of the hydrological model estimation results. NSE values are in the interval of -∞ to 1. The closer the result is to 1, the better the model fitting effect is. The mathematical formula is shown below:

$$E = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y}_i)^2}, \tag{11}$$

where $\hat{y}_i$ is the simulated runoff, and y_i represents the observed runoff.

4. RESULTS

4.1 Monthly Runoff Simulation Results

First, the distributed hydrological model HIMS was calibrated and verified, and take the highest temperature, lowest temperature and precipitation of three meteorological stations as inputs to simulate runoff, as shown in Figure 3 (a). The simulated runoff is used as the output of the physical model.
To facilitate comparison, the same input as HIMS is selected as the input of the LSTM model to simulate runoff, as shown in Figure 3 (b). The simulated runoff is used as the output of the data-driven model.
To facilitate comparison, the preliminary runoff estimation Q' of HIMS and the highest temperature, lowest temperature and precipitation of three meteorological stations are taken as the driving factors, and the estimation is carried out under the condition of ensuring the same input data as HIMS and LSTM, as shown in Figure 3 (c). The simulated runoff is used as the output of the hybrid model.
The evaluation indexes of different models are shown in Table 1. The R^2 of the HPD model is 0.969, which is 1.36% and 3.09% higher than that of HIMS and LSTM respectively; NSE was 0.969, increased by 0.83% and 5.10% respectively; The corresponding RMSE is 13.105, reduced by 15.36% and

27.98% respectively, indicating that the HPD model has the best effect in runoff estimation. According to the model principle, the HPD model combines the advantages of a physical model and a data-driven model, so that the estimated value will not deviate too much. The complex features are extracted from the deep learning model to learn and make up for the systematic differences in the hydrological model.

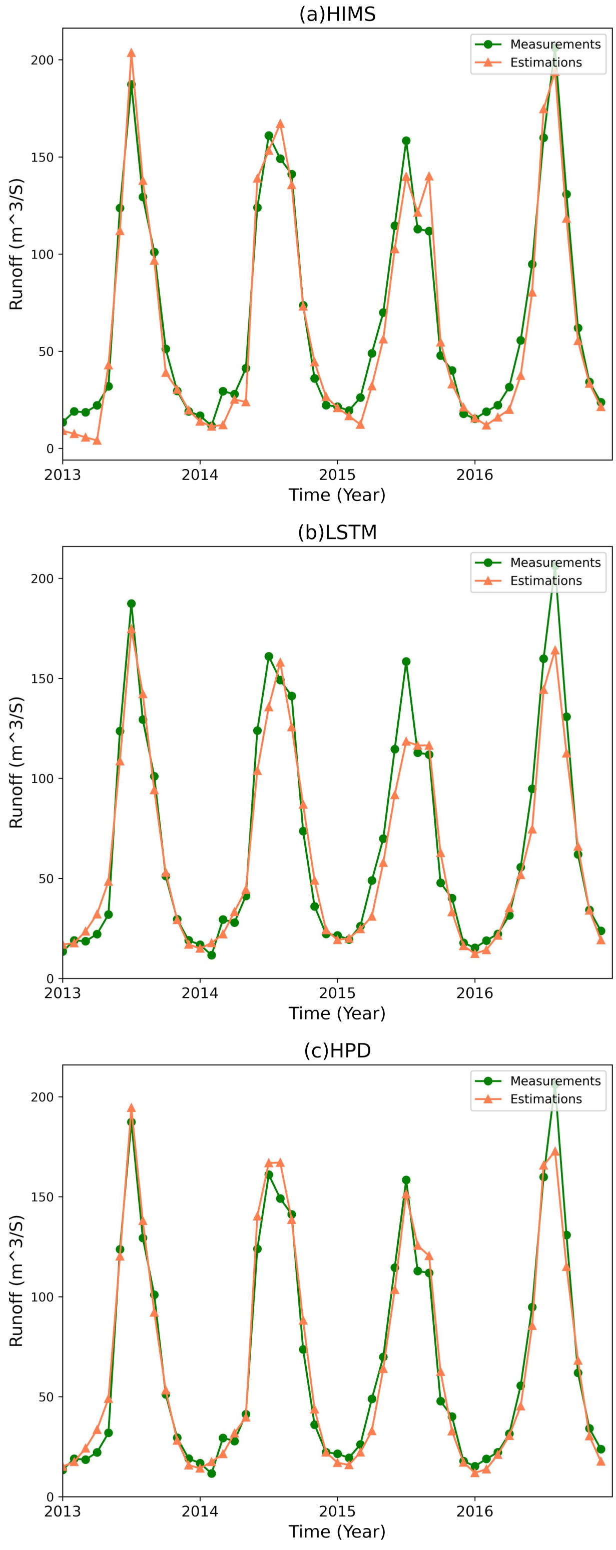

Figure 3. three kinds of runoff estimation.

Input	R^2	RMSE	NSE
HISM	0.956	11.395	0.961
LSTM	0.940	13.392	0.922
HPD	0.969	9.645	0.969

Table 1. monthly runoff simulation.

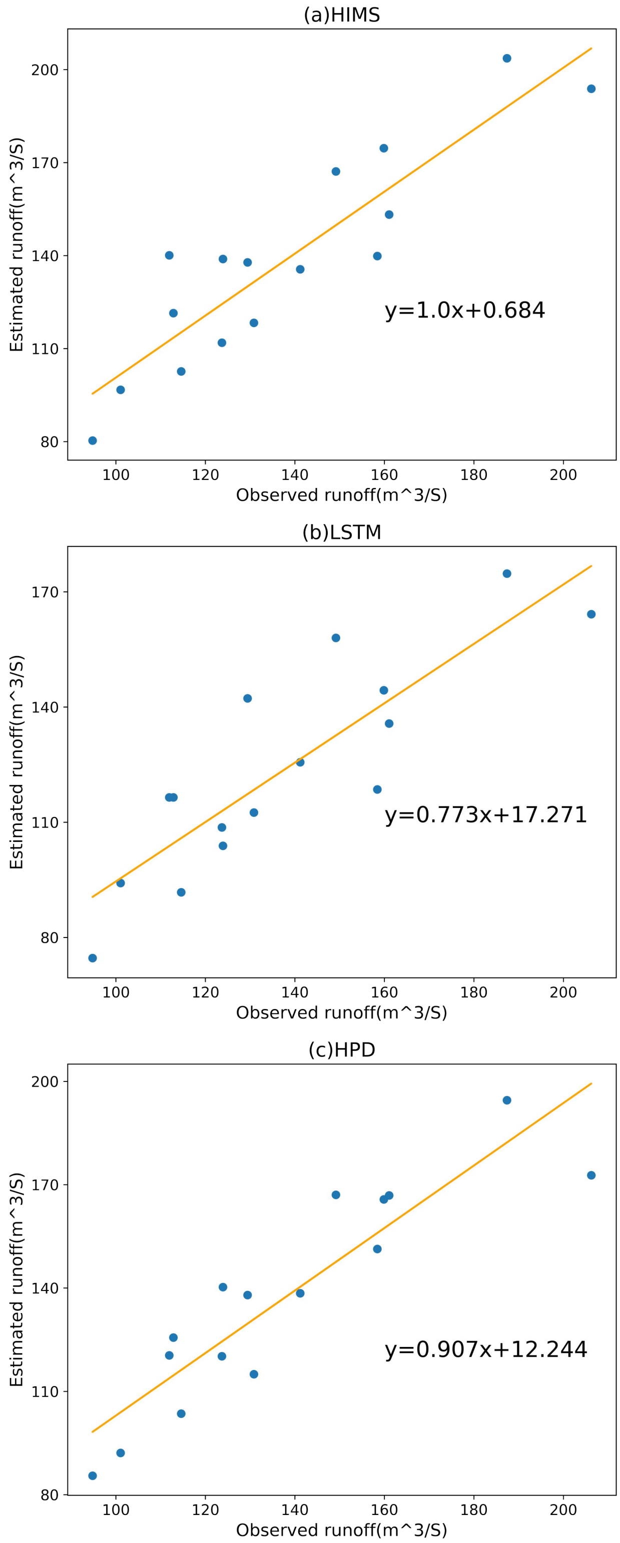

Figure 4. three kinds of runoff estimation in flood period.

https://doi.org/10.5194/isprs-annals-V-3-2022-347-2022

Input	R^2	RMSE	NSE
HISM	0.774	14.208	0.815
LSTM	0.520	20.706	0.404
HPD	0.808	13.105	0.809

Table 2. runoff simulation in flood period.

For the optimal LSTM model, the number of neurons in each hidden layer is 40, the number of training iterations is 15000, and the learning rate is 0.0002. The dropout regularization method was used to prohibit overfitting, and the value is set to 0.5.
For the optimal HPD model, the number of neurons in each hidden layer is 40, the number of training iterations is 10000, the learning rate is 0.001, and the dropout is set to 0.5.

4.2 Runoff Simulation Results in Flood Period

It is notoriously difficult to estimate flood peaks using runoff estimation models. Therefore, we performed additional evaluations of the estimates during the flood period (June to September each year) to assess the model's performance in estimating peak runoff, as shown in Figure 4.
Evaluation indexes of different models are shown in Table 2. It can be seen that the LSTM model has the worst effect in flood peak simulation, which to some extent illustrates one of the drawbacks of LSTM models. Although they have unique features in time series processing, they still have shortcomings in extreme point estimation. HPD model has the best estimation result, with R^2 and NSE values as high as 0.808 and 0.809, respectively, and RMSE values as low as 13.105. This further confirms that the HPD model can make the estimated runoff closer to the real value, which is more obvious in the estimation of flood peak.

5. DISCUSSION

In this letter, the hybrid physical data model we adopted only preliminarily combines the deep learning with the physical model, and we have to make further efforts to integrate the physical knowledge into the deep learning model. For example, the P-RNN layer of the hydrology-aware deep learning model developed by Jiang is wrapped with physically meaningful parameters in physical model(Jiang et al., 2020). Additionally, some studies regard the physical constraints as loss terms in the neural networks, and have been successful in some fields(Karpatne, Watkins et al., 2017; Read et al., 2019).
In this letter, for the convenience of the experiment, the physical hydrological model we selected is only a simplified version, only using the simplest data for runoff simulation, so the simulation accuracy may not reach the upper limit of the HIMS model. If more comprehensive inputs are used, the HIMS model's estimation accuracy will be higher, and accordingly, the HPD model's estimation accuracy will be improved.
In addition, one reason why we build the hybrid model is to obtain physically consistent estimation results. However, some experts believe that the randomness of training weights injected into neural networks during dropout is enough to eliminate the physical consistency caused by the physics-guided loss during training(Karpatne, Watkins et al., 2017). Therefore, we should also consider that the dropout method is physically inconsistent with the estimation results while enhancing the generalization ability of the model.

6. CONCLUSIONS

In this letter, a hybrid physical data model combining physical model and deep learning model is established. More specifically, the output of a physically hydrological model HIMS used as another input in the neural network model along with the drivers. The following results are obtained.
1. HPD model has an excellent learning capability to simulate runoff and a flexible ability to extract complex relevant information. Using the HPD model results in high R^2, and NSE values of 0.969, respectively, and a low RMSE value of 9.645.
2. It can be seen from Table 2 that the HPD model has a good improvement on flood peaks simulation. Flood period simulation results in high R^2, and NSE values of 0.808 and 0.809 , respectively, and a low RMSE value of 13.105.
The method of combining the physical model with the deep learning model can effectively improve the accuracy of the model, which proves the applicability of the mixed physical data model in runoff estimation. The HPD model is effective in estimating the general trend of runoff and tracking the extreme value. The results can provide a reference for water resources management and scientific decision-making in the study area.

7. ACKNOWLEDGEMENTS

This work was supported by the National Natural Science Foundation of China (No. 42061056), the Doctoral Foundation of Henan Polytechnic University under Grant B2017-09, the Major Science and Technology Program of Henan Province (No. 222102320341), the Key Scientific Research Project in Colleges and Universities of Henan Province (No. 22B420004), and the Fundamental Research Funds for the Universities of Henan Province (No. NSFRF210401).

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