

Research Progress and Prospect of Hydrological Models Coupling Mechanism-Driven and Data-Driven Approaches

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Abstract. Under the combined impacts of climate change and intensive human activities, watershed water circulation exhibits obvious non-stationarity, nonlinearity and cross-scale coupling characteristics. Both traditional mechanism-driven hydrological models and data-driven models are confronted with new challenges in applicability. The former can explicitly describe hydrological processes and possess good interpretability, yet it is often restricted by problems including parameter identifiability, structural errors and scale conversion. The latter is capable of learning complex mapping relationships from large-scale and multi-source datasets, and performs well in runoff forecasting, flood simulation and prediction in ungauged basins. Nevertheless, it suffers from insufficient physical consistency, extrapolation risks and poor mechanistic interpretation. In recent years, the rapid development of methods such as physically constrained machine learning, differentiable hydrological models, neural network regionalization of parameters, model post-processing and cross-model integration has promoted the transformation of hydrological models from the simple choice between mechanism and data to data learning under physical constraints. This paper systematically reviews the research progress of mechanism-driven models, data-driven models and their integration paradigms, compares the applicable scenarios and limitations of different integration routes, and proposes future research directions in terms of multi-source remote sensing data assimilation, cross-regional generalization, extreme event prediction, uncertainty quantification and the construction of digital twin watersheds.

Keywords: hydrological model, mechanism-driven model, data-driven model, physically constrained machine learning, differentiable modeling

1. Introduction

Hydrological models serve as essential tools for understanding watershed runoff generation and concentration processes, and supporting flood forecasting, water resources regulation, drought risk assessment as well as impact analysis of climate change. Classical models generally abstract complex water circulation processes into empirical formulas, conceptual reservoirs or distributed physical equations based on water balance, energy balance, underlying surface runoff generation mechanisms and river network concentration rules. Representative models including TOPMODEL, VIC, SWAT, the GR series, Xin'anjiang Model and various land surface hydrological models all follow the fundamental principle of "interpreting watershed responses via process structures" [1-4].

This modeling approach features clear physical implications, and facilitates scenario analysis and interpretation for management. Nevertheless, its performance heavily relies on model structural assumptions, parameter calibration quality and input data accuracy, and tends to generate structural biases under non-stationary climate, urbanization, irrigation, reservoir operation and other intensive human activities [5, 6].

In contrast, data-driven models focus on learning the nonlinear relationships between inputs and outputs from observational data. With the development of large-scale watershed datasets, remote sensing products, reanalysis data and deep learning frameworks, long short-term memory (LSTM), convolutional neural networks, graph neural networks and Transformer-based models have been widely applied to rainfall-runoff simulation and runoff forecasting [7-11]. In particular, LSTM models trained through cross-basin joint training have achieved better predictive performance than traditional conceptual models on many public benchmark datasets [8, 12]. However, pure data-driven models often fail to guarantee water balance and physical consistency, and may produce unreliable extrapolation results when applied to extreme events, ungauged areas and climate change scenarios [9, 10].

Accordingly, the core trend of current hydrological model research is not to simply replace mechanism-based models with artificial intelligence, but to explore in-depth integration of the two. On one hand, mechanism-driven models provide prior structures, state variables and physical constraints to reduce the risk of unconstrained fitting in machine learning. On the other hand, data-driven approaches are adopted to correct structural errors of traditional models, simulate subgrid processes that cannot be explicitly expressed, and improve model efficiency for large-sample datasets, multi-region applications and real-time operational scenarios.

1.1. From empirical models to distributed process models

All mechanism-driven models are built on the theory of water balance. Within a given spatio-temporal unit, precipitation, evapotranspiration, surface runoff, subsurface runoff and variations in water storage satisfy the basic conservation principle, which can be simplified as the formula: $P - ET - Q - \Delta S = 0$. Early empirical models mostly describe watershed responses using statistical relationships or unit hydrograph methods. They are easy to calculate but incapable of revealing internal hydrological processes. Conceptual models further abstract a watershed into multiple reservoirs and threshold functions, and simulate soil water storage, runoff generation and concentration with a small number of parameters. Distributed models adopt grid data including digital elevation models, land use, soil, vegetation and meteorological data to characterize the spatial heterogeneity of underlying surfaces. The main characteristics of different model categories are presented in Table 1.

Table 1. Comparison of characteristics of major hydrological model types

Model Type	Representative Methods or Models	Major Advantages	Major Limitations
Empirical/Statistical Models	Unit hydrograph models, regression models, time series models	Simple structure, few parameters, and easy operational implementation	Limited extrapolation capability and weak representation of physical processes

Table 1. (continued)

Conceptual Models	TOPMODEL, GR4J, Xinanjiang model, etc.	Balance computational efficiency with hydrological realism; well suited for streamflow forecasting	Pronounced parameter equifinality and structural errors
Distributed Physically Based Models	VIC, SWAT, land surface hydrological models, etc.	Capture spatial heterogeneity and support scenario analysis	High data requirements, complex calibration, and substantial computational cost
Land–Atmosphere/Hydrological Coupled Models	Land surface process models, hydrological–hydrodynamic coupled models	Well suited for climate change studies and regional water cycle simulations	Complex scale transformation and uncertainty propagation

1.2. Advantages and bottlenecks of mechanism-driven models

The greatest merit of mechanism-driven models lies in the capability to correlate model outputs with actual hydrological processes. For flood forecasting, for instance, the models can not only produce discharge hydrographs, but also track state variables such as soil moisture content, evapotranspiration, snowmelt, groundwater recharge and river routing. For scenario analysis concerning climate change and human activities, the models can assess the direction and magnitude of watershed responses by adjusting parameters related to precipitation, temperature, land use, irrigation and reservoir operation rules. Such interpretability makes mechanism-driven models irreplaceable for water resources management and engineering decision-making.

Even so, mechanism-driven models have long been restricted by three major bottlenecks. The first is parameter identifiability. Most parameters cannot be directly observed and have to be inversely estimated from limited outputs such as runoff, which leads to the equifinality problem where different parameter combinations yield similar simulation results. The second is structural errors. Simplified descriptions of runoff generation, evapotranspiration, infiltration, snowmelt and human regulation processes in models cannot fully reflect the complexity of real-world watersheds. The third is scale-related issues. When formulas applicable to plot-scale experiments are directly applied to watershed-scale research, biases will arise due to neglected spatial heterogeneity and subgrid processes. These defects mean that traditional mechanism-driven models require new technical support for applications in ungauged areas, extreme event simulation and non-stationary environments.

2. Data-driven hydrological models: from machine learning to hydrological deep learning

2.1. Traditional machine learning and deep learning methods

Data-driven models have evolved from traditional machine learning approaches including linear regression, support vector machine, random forest and gradient boosting decision tree to deep learning methods such as LSTM, convolutional neural network, graph neural network and Transformer. Traditional machine learning performs well with small and medium-sized datasets, and is applicable to tasks with definite feature variables and moderate nonlinearity. In contrast, deep learning can automatically extract temporal dependencies and spatial features, and shows excellent performance in watersheds with long-term memory, water-snow transformation processes and multi-source data fusion. Kratzert et al. [8] adopted LSTM for rainfall-runoff simulation, and verified that this network can capture the water storage effect of watersheds from meteorological inputs,

achieving accuracy equivalent to or higher than that of classical models. Since then, training with large-scale watershed datasets has become a major paradigm of hydrological deep learning.

Compared with single-basin training, joint training across multiple basins enables models to learn generalized hydrological behaviors from differences in climate, terrain, soil and vegetation conditions. Kratzert et al. [12] further pointed out that LSTM-based rainfall-runoff models are not suitable for training on a single basin only, because shared information contained in cross-basin samples helps improve model generalization ability. This viewpoint has promoted the development of open datasets such as CAMELS and Caravan, as well as tools including NeuralHydrology [5, 11]. Meanwhile, hydrological modeling has gradually shifted from single-station calibration to regional learning based on large datasets.

2.2. Limitations of data-driven models

Despite the prominent advantages in prediction accuracy, the scientific application of data-driven models still faces three major challenges. First, the internal states of models may not correspond to real hydrological variables, and the black-box nature reduces the credibility of model outputs in management and decision-making. Second, these models are sensitive to the distribution of training data, and may produce uncontrollable extrapolation results when encountering extreme precipitation, unprecedented drought or drastic changes in human regulation activities. Third, the models may violate fundamental principles such as water balance. For instance, if there are systematic errors in precipitation input, pure data-driven models can still attain favorable statistical indicators through empirical compensation, yet the interpretation of internal processes remains unreliable. To address these issues, mass conservation networks, physically constrained loss functions and interpretable deep learning have been proposed to strike a balance between prediction performance and physical consistency [10, 13].

3. Integration paradigms of mechanism-driven and data-driven hydrological models

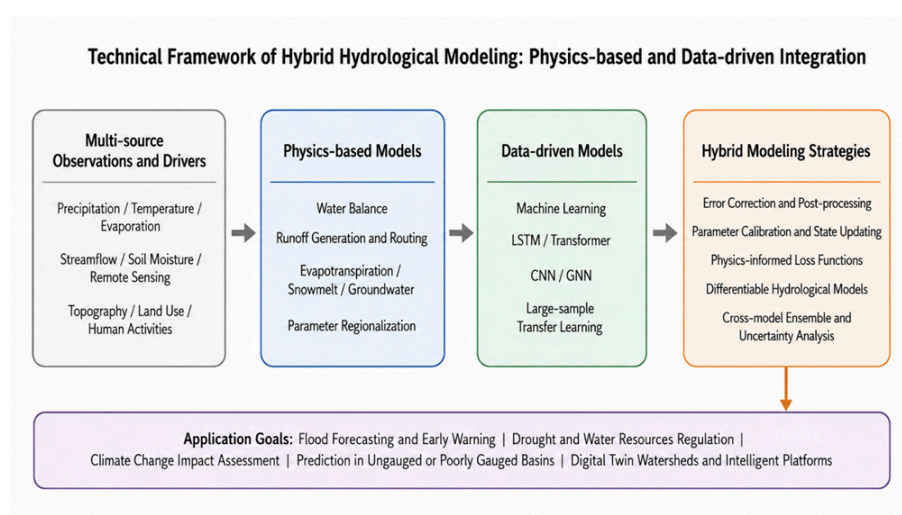


Figure 1. Technical framework of hydrological models integrating mechanism-driven and data-driven approaches

Current studies on model integration are generally classified into four categories: post-processing of model outputs, machine learning assisted parameter calibration and regionalization, physically

constrained or physics-informed deep learning, and end-to-end coupling between differentiable mechanism models and neural networks. These approaches are not mutually exclusive, and can be combined according to data availability, application objectives and operational constraints. Figure 1 illustrates the basic logic from multi-source observation data and integrated modeling to practical application targets.

3.1. Integration via post-processing and error correction

The most straightforward integration method takes mechanism-driven models as basic predictors, and adopts statistical or machine learning methods to correct their systematic biases. To be specific, process-based models first simulate discharge, evapotranspiration or soil moisture, and then errors are corrected by random forest, LSTM, quantile mapping or generalized linear models. Slater et al. [14] defined this strategy as hybrid forecasting, where data-driven models are used to integrate forecast information from numerical weather, climate, land surface and hydrological dynamic models. A 2025 study on large-scale hydrological models across Europe indicated that post-processing with machine learning can effectively improve the simulation of local runoff and extreme discharge. Nevertheless, different post-processing methods present spatial complementarity, and no single approach performs optimally for all regions [15]. This method features low engineering implementation cost and is suitable for operational forecasting. However, its physical interpretation is limited to model outputs, and it barely improves the internal processes of original models.

3.2. Parameter regionalization and model structure replacement

The second type of integration applies machine learning to estimate parameters of mechanism-driven models, or replaces internal modules that cannot be accurately formulated with neural networks. This framework retains the water balance and state evolution rules of original models, while neural networks learn the complex relationships between parameters and watershed attributes, meteorological conditions or internal model states. In recent years, embedded neural networks (ENNs) have been employed to replace modules for evapotranspiration, snowmelt, runoff generation and flow concentration. Research on large watersheds over the Qinghai-Tibet Plateau shows that taking semi-distributed process models as the main framework and adopting ENNs to parameterize or replace partial internal modules can maintain explicit hydrological knowledge, while achieving accuracy comparable to state-of-the-art deep learning models [16]. The latest distributed hybrid frameworks further utilize machine learning to correct internal hydrological fluxes, enhancing the capacity for regional flood simulation at high spatial resolution [17]. Such methods are especially applicable to alpine mountainous areas, irrigation districts, urban watersheds and other regions with prominent structural errors, where process interpretation is still required.

3.3. Physically constrained deep learning and differentiable hydrological models

Differentiable hydrological models represent the most rapidly developing direction in recent years. The core idea is to convert equations governing runoff generation, evapotranspiration, snowmelt and flow concentration in mechanism-driven models into computation graphs supporting automatic differentiation. Neural networks are then embedded for parameter estimation, state updating or expression of unknown processes, and end-to-end training is realized via back propagation. Feng et al. [18] verified that differentiable physics-informed models with regionalized deep network parameterization have great potential for ungauged basins and climate change scenarios. Afterwards,

studies such as δ HBV-globe1.0-hydroDL extended differentiable models to 3753 watersheds worldwide, setting a new benchmark for large-scale hydrological simulation [19]. Wang et al. [20] established a physics-encoded deep learning framework for the Amazon Basin, proving the feasibility of joint training for distributed hydrological models and neural networks.

Differentiable modeling unites the structural constraints of mechanism-driven models and the parameter learning capability of deep learning within one optimization framework. It not only improves the accuracy of runoff prediction, but also enables the output of variables without direct supervision, including evapotranspiration, soil moisture and groundwater recharge. The release of SMASH v1.0 in 2025 further demonstrates that differentiable, regionalizable and high-resolution hydrological modeling frameworks are evolving toward scientific research and operational application [21]. In China, relevant researches on differentiable transformation based on the Xin'anjiang Model have also emerged. The dXAJ model retains the structure of the Xin'anjiang Model and introduces LSTM for parameter learning, providing a localized solution for integrating traditional watershed models with deep learning [22].

3.4. Comparison of integration approaches

Table 2. Comparison of major integration approaches for hybrid mechanism-data hydrological models

Integration Pathway	Technical Implementation	Typical Applications	Key Risks
Output Post-processing	Apply RF, LSTM, QM, or other methods to correct the outputs of process-based models	Operational forecasting, local bias correction, and rapid deployment	Can improve predictive accuracy but offers limited process interpretability
Machine Learning-Based Parameter Calibration	Predict model parameters from watershed characteristics or dynamic meteorological conditions	Ungauged basins, parameter regionalization, and multi-basin learning	The physical meaning of model parameters may be weakened
Internal Module Replacement	Replace evapotranspiration, snowmelt, runoff generation, or other process modules with neural networks	Applications with significant structural errors while retaining the underlying model framework	Excessive replacement may transform the model into a black-box system
Physics-Constrained Learning	Incorporate water balance, boundary conditions, or governing process equations into the loss function	Tasks requiring physical consistency and robust extrapolation	Inaccurate constraints may limit model performance
Differentiable Models	Construct differentiable computational graphs by integrating process-based equations with neural networks	Large-sample training, data assimilation, and end-to-end optimization	Complex implementation, high computational cost, and immature evaluation frameworks
Cross-Model Integration	Combine LSTM, δ HBV, process-based models, and multiple meteorological forcings	Improve generalization capability and uncertainty quantification	Complex model selection and challenging interpretation of uncertainties

It should be noted that incorporating physical knowledge does not necessarily lead to performance improvement (Table 2). In 2026, Álvarez Chaves et al. [13] proposed an entropy-based method to evaluate the respective contributions of physical constraints and data-driven components in hybrid models. The results indicate that when the conceptual structure fails to match real hydrological processes, neural networks may adjust parameters to bypass original physical

constraints. In extreme cases, the so-called physical constraints will become a burden for prediction. This finding suggests that the development of integrated models should not merely pursue advanced structures; it is more critical to verify whether physical constraints can function effectively.

4. Application fields and future development trends

4.1. Typical application fields

First, flood forecasting and extreme event simulation are the most practically demanded directions for integrated models. Mechanism-driven models can reflect runoff generation under rainstorm and river routing processes, while deep learning excels at identifying nonlinear precursors and temporal memory from historical data. Studies on glacier and snowmelt watersheds have proven that combining outputs of cryosphere hydrological models with CNN-LSTM and wavelet transform can markedly improve the prediction accuracy of high flow [23]. Second, drought monitoring and water resources regulation require comprehensive analysis of evapotranspiration, soil moisture, groundwater and human water use, and simple runoff fitting by a single model can hardly meet management requirements. Integrated models can incorporate remotely sensed evapotranspiration, soil moisture and total water storage changes into model training or data assimilation, so as to enhance the consistency of multiple variables. Third, impact assessment of climate change and prediction in ungauged basins demand strong cross-regional extrapolation capability. Differentiable models and cross-model ensembles show great potential in this regard. Particularly for spatial extrapolation and prediction in unobserved areas, structural constraints can deliver stability that pure data-driven models fail to achieve [18, 19, 24].

4.2. Future development trends

Future research can be further advanced in five aspects. Firstly, establish a unified evaluation system for multi-variable water circulation. Evaluating model performance merely with NSE or RMSE based on runoff is no longer sufficient for integrated models. It is necessary to comprehensively assess water balance, evapotranspiration, soil moisture, groundwater, extreme flow, low flow and model uncertainty. Secondly, strengthen the assimilation and utilization of remote sensing and reanalysis data. Remote sensing can provide spatially continuous information on evapotranspiration, snow cover, vegetation, soil moisture and surface water bodies, which serves as a key solution to the problem that models are only constrained by outlet discharge observations. Thirdly, develop interpretable physically constrained machine learning. Models are required not only to achieve accurate prediction, but also to clarify which hydrological processes are revised, which parameters are altered, and whether such changes conform to hydrological theories. Fourthly, conduct extrapolation tests targeting non-stationary climate and human activities. Future climate conditions, land use changes, irrigation and reservoir operation should be incorporated into the model training and validation framework, instead of comparing accuracy only under historical data with identical distribution. Fifthly, build open and reproducible artificial intelligence platforms for hydrology. Open-source tools including NeuralHydrology, SMASH and δ HBV indicate that standardized datasets, codes and benchmark experiments will lay a solid foundation for high-quality development of this research field [11, 19, 21].

5. Conclusions

In general, mechanism-driven models and data-driven models are two complementary paradigms in hydrological science. The former focuses on process understanding, physical consistency and scenario interpretation, while the latter aims to learn complex nonlinear relationships from multi-source data and improve prediction performance. Recent studies reveal that the integration of the two has evolved from simple error correction to parameter regionalization, internal module replacement, physically constrained deep learning, differentiable hydrological models and cross-model ensemble. A high-performance integrated model cannot be realized by mechanically embedding neural networks into traditional models. Instead, it is essential to define the applicable scope of physical constraints, diagnose the compensation mechanism of data-driven components, and verify model reliability through multi-variable, multi-scale and multi-scenario evaluation. For future hydrological modeling, the most promising direction is to develop a new generation of intelligent hydrological model system featured with reliable physical mechanisms, sufficient data support, diagnosable structures, interpretable results and reproducible platforms.

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