Towards HydroLLM: Building a Domain-Specific Language Model for Hydrology

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Abstract

As large language models (LLMs) continue to expand, their effective adaptation to specialized fields remains a critical challenge. This work presents an initial step toward the development of HydroLLM, a domain-specific LLM for hydrology. We construct a dataset of approximately 8,800 hydrology-focused question–answer pairs, each with a supporting context passage drawn from textbooks and scientific articles. The dataset includes four instructional formats: multiple choice, true/false, fill-in-the-blank, and open-ended. Using this corpus, we fine-tune several LLMs of varying type and scale—from compact (1.5B) to large (32B) parameter counts using parameter-efficient LoRA (Low-Rank Adaptation) methods. Our methodology compares different fine-tuned models and evaluates model performance using accuracy and cosine similarity metrics across task types. Results show that larger model size is not always advantageous: among the fine-tuned models, the 8B DeepSeek Llama variant achieved the strongest overall performance, while the 32B model overfit and the 1.5B model underperformed—emphasizing the need to match model capacity to dataset size. This work demonstrates that effective domain adaptation requires careful consideration of model architecture, parameter count, and task complexity, with fill-in-the-blank tasks proving particularly challenging across all models. By establishing performance and identifying the limits of current fine-tuning approaches, we took a concrete step toward building HydroLLM as a robust, domain-specific language model for hydrological analysis and decision support.

Keywords: HydroLLM, Large Language Models (LLMs), Fine-Tuning, Hydrology, Question Generation, Domain-Specific AI, Natural Language Processing (NLP)

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1. Introduction

Hydrology is the study of water's distribution, movement, and properties across the Earth's surface, subsurface, and atmosphere. As a core environmental discipline, it provides a critical foundation for understanding the hydrologic cycle, including processes such as precipitation, evaporation, infiltration, runoff, and how these processes interact with ecological and human systems (Vogel et al., 2015; Pierrehumbert, 2002). The field is inherently interdisciplinary, drawing from geophysics, environmental science, and engineering to inform water-related decision-making in agriculture, infrastructure (Alabbad et al., 2024), climate resilience (Tanir et al., 2024), and disaster risk reduction (Ding et al., 2015; Weinmann, 2007).

In a world facing increasing water stress, climate variability, and rapid land-use change, hydrology plays a vital role in managing freshwater resources sustainably (Demir et al., 2022). This includes studies to monitor water availability, assess environmental risks, and guide adaptive planning strategies (Sit et al., 2021). Despite its maturity as a scientific field, hydrology continues evolving through integration of modern technologies and data-driven approaches, particularly in developing climate-based assessment frameworks (Keller et al., 2023). This evolution emphasizes hydrology's central role in comprehensive water resources management (Bonacci, 2004). National benchmark datasets and monitoring networks now support more evidence-based decision-making (Wilford et al., 2010). Deep learning methods represent a promising frontier, showing potential for prediction and classification tasks that contribute to long-term water security (Sit et al., 2022).

Hydrology, despite its longstanding scientific foundation, continues to grapple with systemic gaps that limit progress in understanding and managing water systems (Blöschl et al., 2019). Core theoretical challenges include the lack of shared perceptual models for regional hydrology, incomplete knowledge of hydrological causality across spatial and temporal scales, and limited understanding of feedback mechanisms between natural and anthropogenic processes (Wagener et al., 2021). Many hydrological models rely on simplifications that fail to capture the heterogeneity of real-world watersheds, especially in urban environments where building structures impose conveyance restrictions and storage characteristics that are inadequately represented in coarse resolution models (Vojinovic et al., 2013), while socio-hydrological frameworks often lack interdisciplinary depth and operational integration (Vanelli et al., 2022; Loch et al., 2014). These conceptual limitations are exacerbated by persistent issues in hydrological data (Demir and Szczepanek, 2017).

Observational networks remain unevenly distributed, especially in the Global South, and subsurface processes remain particularly difficult to monitor with precision (Beven et al., 2020; Baydaroglu et al., 2024). These data limitations are notably pronounced in developing countries, where insufficient hydro-meteorological data significantly hinders effective disaster management strategies, though recent methodological advances have demonstrated that parameter sensitivity analysis combined with digital elevation model modifications can provide viable solutions for urban flood modeling under such data-scarce conditions (Dasallas et al., 2024). Beyond data scarcity, the integration of heterogeneous data sources — ranging from in-situ measurements to

satellite-derived estimates — is constrained by inconsistent formats, temporal resolution mismatches, and weak standardization (Lehmann et al., 2014; Oswald et al., 2024).

To address these integration challenges, knowledge graph approaches have emerged as promising solutions for bridging data silos in water quality assessment, enabling the integration of multiple segregated data sources to provide interoperable views that combine physicochemical, biological, spatio-temporal, and regulatory information (Rondón Díaz & Vilches-Blázquez, 2022). Data quality assessment in hydrological information systems remains especially challenging, as hydrological data may be compromised by network congestion, instrument failures, and human errors. This requires comprehensive quality management approaches that extend beyond traditional intrinsic quality problems to assess data utility within specific application contexts (Chao et al., 2015). Even in data-rich regions, uncertainty in precipitation inputs, evapotranspiration estimates, and soil moisture datasets introduce significant noise into model outputs (Singh et al., 2024), presenting considerable challenges for real-time urban flood forecasting systems that must operate under accepted flood risk conditions while providing timely predictions despite data uncertainties (Henonin et al., 2013). While machine learning and novel Earth observation technologies have made inroads, their effectiveness is often limited by data scarcity, low representativeness, and challenges in generalizing across hydrological regimes (Zhong et al., 2024).

Taken together, these challenges underscore the urgent need for new tools and frameworks that can bridge data fragmentation, capture local context, and support scalable analysis across hydrological systems. Addressing these bottlenecks — particularly those rooted in data access, integration, and contextual interpretation — is a necessary step toward advancing both predictive modeling and informed decision-making in hydrological science (Pursnani et al., 2025).

The integration of artificial intelligence (AI) techniques has emerged as a transformative approach for addressing many of these hydrological challenges. Machine learning and deep learning methods, including artificial neural networks and recurrent neural networks, have demonstrated exceptional performance in modeling complex hydrological processes such as rainfall-runoff, streamflow, and groundwater dynamics (Poonia et al., 2018; Karunarathna & Rajapakse, 2024; Krajewski et al., 2021). Convolutional neural networks (CNNs) have also shown particular promise in rainfall-runoff modeling, with studies demonstrating their ability to capture nonlinear relationships and exploit correlation structures in multivariate time series data while requiring shorter historical records compared to traditional recurrent networks (Van et al., 2020).

Similarly, wavelet-based long short-term memory (WLSTM) models have demonstrated superior performance in river stage prediction tasks, particularly for capturing peak stage values and data periodicities through noise reduction, making them valuable tools for flood early warning systems (Chakraborty & Biswas, 2024). AI applications have proven particularly valuable in water resource management, providing accurate predictions for flood modeling, drought conditions, and water quality assessments, especially in data-scarce regions (Kambarbekov & Baimaganbetov, 2024; Zekrifa et al., 2023). Advanced machine learning models, including XGBoost and LSTM networks, have demonstrated exceptional performance in water quality prediction and

classification tasks, achieving near-perfect accuracy rates and superior generalization capabilities when handling complex, multivariate water quality datasets (Elmotawakkil et al., 2025).

Data-driven modeling frameworks have also shown significant promise in municipal water system management, with machine learning approaches successfully predicting system responses to hydroclimate extremes and accurately classifying vulnerability scenarios, offering computationally efficient alternatives to complex systems models (Johnson et al., 2023). In agricultural water management, machine learning techniques including random forest, artificial neural networks, and support vector machines have demonstrated superior predictive accuracy for evapotranspiration estimation and water stress prediction, with the integration of real-time data streams from satellite imagery and climatic variables enhancing precision in water management strategies (Mortazavizadeh et al., 2025).

These capabilities are further enhanced by comprehensive cyberinfrastructure systems that integrate data analytics, visualization, and communication platforms for flood and drought management, supporting both operational forecasting and public awareness initiatives (Yeşilköy et al., 2024). Additionally, AI-driven decision support systems have demonstrated effectiveness in enhancing collaborative planning processes, with multi-agent frameworks showing promise in flood mitigation and water resource management through improved stakeholder engagement and strategic optimization (Kadiyala et al., 2024a). Furthermore, AI-augmented frameworks have enhanced automation in model conceptualization and execution, democratizing advanced hydrological modeling for researchers worldwide (Eythorsson & Clark, 2025). However, challenges remain regarding model interpretability, data quality dependencies, and the need for explainable AI tools to provide insights into underlying physical mechanisms (Slater et al., 2024; Muñoz-Carpena et al., 2023).

Recent advances in large language models (LLMs) have catalyzed transformative progress across scientific disciplines—including biology, chemistry, and medicine—through their ability to parse complex texts, synthesize literature, and support problem-solving in domain-specific contexts (Zhang et al., 2025; AI4Science & Quantum, 2023). In hydrology and environmental sciences, the application of LLMs is expanding rapidly, with significant growth in LLM-based studies, especially in hydrological modeling, climate forecasting, and environmental monitoring (Sajja et al., 2025). Early efforts have demonstrated their utility in tasks ranging from literature analysis to real-time environmental monitoring. For example, WaterGPT, a domain-adapted LLM, has shown promise in processing both textual and visual hydrological data to extract information on reservoir operations, waterbody detection, and document classification (Ren et al., 2024; Yang et al., 2024). LLM-enhanced platforms such as HydroSuite-AI have further demonstrated the potential of integrating language models with hydrological libraries to facilitate code generation, documentation assistance, and workflow automation for researchers (Pursnani et al., 2024).

Conversational AI agents have also shown promise in water quality education and management, with LLM-based systems achieving high accuracy in delivering contextually relevant information for community engagement and environmental conservation efforts (Samuel et al., 2024). Similarly, multimodal LLMs (MLLMs) such as GPT-4 Vision have been applied to

flood management and water level estimation by interpreting satellite imagery and ground data, providing timely insights for operational decision-making (Kadiyala et al., 2024b). Recent work has also explored the capacity of large language models to provide reasoning on adverse weather conditions and classify official hazard reports. For example, Zafarmomen and Samadi (2025) systematically evaluated the performance of several LLM architectures—including BART, BERT, LLaMA-2, LLaMA-3, and LLaMA-3.1—on the task of classifying flood reports from the US National Weather Service. Their findings highlighted the potential and limitations of LLMs in handling imbalanced disaster datasets and recognized the importance of adapting fine-tuning approaches, such as LoRA, for improved performance.

Despite these advances, general-purpose models often fall short when applied to hydrology-specific tasks. Challenges include poor adaptation to technical vocabulary, limited access to domain-aligned corpora, and a lack of standardized benchmark datasets for robust evaluation (Rostam & Kertész, 2024; Acharya et al., 2024). These issues are compounded by broader problems in scientific LLM development, such as the trade-off between generalization and in-domain expertise, as well as the computational demands of domain-specific fine-tuning (Chen et al., 2024; To et al., 2024). Traditional ensemble modeling approaches using neural networks have demonstrated the value of multi-model integration in hydrological simulations (Li et al., 2018). Building on this foundation, multi-model approaches that combine the outputs of traditional hydrological models like SWAT or VIC with LLM-driven interpretations have shown promise in improving prediction accuracy and integrating physical insights with machine learning flexibility, particularly for climate change impact assessment and operational decision-making (Perra et al., 2018).

In this paper, initial efforts toward developing HydroLLM are presented along with insights and recommendations in the path for artificial general intelligence (AGI) for hydrology. Rather than introducing a finalized architecture, we conduct a series of targeted fine-tuning experiments using a curated dataset of hydrology-related question–answer pairs. These experiments are designed to probe the capabilities and limitations of current LLMs in handling domain-specific reasoning through fine-tuning under data-limited conditions. Our findings reveal key challenges—such as poor contextual grounding, factual drift, and inconsistency across question types—that highlight critical design considerations for future model development. By identifying these gaps, our study offers concrete insights into the data requirements, evaluation strategies, and adaptation techniques necessary for building effective hydrology-specific language models.

2. Methodology

To guide the development efforts of HydroLLM, we constructed a curated dataset comprising question–answer pairs across multiple formats—multiple choice, true/false, fill-in-the-blank, and open-ended—to capture the instructional and conceptual diversity of hydrological knowledge. Each question was paired with a relevant context passage and a labeled answer to ensure domain grounding and evaluation consistency. The methodology encompasses the overall scope and purpose of our study, the steps involved in dataset creation, and a series of model fine-tuning

experiments using parameter-efficient adaptation techniques. It also details the evaluation framework used to assess model performance, with particular emphasis on accuracy and the contextual relevance of generated outputs.

2.1. Scope and Purpose

The ultimate and long-term vision driving this research is the development of artificial general intelligence (AGI) capabilities specifically tailored for hydrology—a system that can reason about complex water systems, integrate diverse data sources, and provide expert-level insights across the full spectrum of hydrological challenges. Such a system would revolutionize how we approach water resource management, flood prediction, drought analysis, and climate adaptation by combining the reasoning capabilities of advanced language models with deep domain expertise. An AGI for hydrology would serve as an intelligent assistant capable of synthesizing vast amounts of hydrological literature, interpreting field observations, generating hypotheses, and supporting decision-making processes that currently require extensive human expertise.

This ambitious goal requires fundamental advances in how we adapt multimodal large language models to scientific domains. Current general-purpose LLMs, while impressive in their broad capabilities, lack the specialized knowledge and reasoning patterns needed for expert-level hydrological analysis. Building toward AGI for hydrology demands understanding how to effectively transfer scientific knowledge, handle domain-specific terminology and concepts, and maintain accuracy in technical reasoning tasks. The challenges are particularly acute in hydrology, where reasoning often involves complex interactions between physical processes, statistical analysis, and practical engineering considerations. The study represents a crucial diagnostic step toward this vision, establishing the foundational empirical understanding necessary for developing truly intelligent hydrological reasoning systems.

2.2. Data Collection and Experimental Setup

This study builds upon our prior work in developing HydroLLM-Benchmark (Kizilkaya et al., 2025), a curated dataset designed to evaluate LLMs on hydrology-specific knowledge. While the original benchmark emphasized breadth across question types and topical coverage, the present work focuses on fine-tuning experiments with different LLMs to identify the key considerations for building an effective HydroLLM.

To ensure domain alignment, we selected two primary source types: (1) the textbook Fundamentals of Hydrology (Davie, 2019), which provides foundational hydrological theory and terminology; and (2) a corpus of 2,000 research articles published between 2022 and 2024 in Journal of Hydrology, Advances in Water Resources, and Journal of Hydrology: Regional Studies. These sources reflect both canonical and contemporary hydrological knowledge.

From these materials, we curated a dataset of approximately 8,800 question–answer (QA) pairs using advanced prompting techniques with GPT-4o-mini. Each QA instance includes a *Context* passage sourced from the text, a *Question* formatted in one of four instructional styles—multiple choice, true/false, fill-in-the-blank, or open-ended—and a *Reference Answer* representing the gold-

standard hydrological interpretation. The inclusion of context is essential not only for grounding model responses but also for enabling evaluations of reasoning fidelity and factual consistency. In contrast to the original benchmark, which was optimized for model evaluation, this new version of the dataset has been systematically created for fine-tuning and model behavior analysis. Specific enhancements include the standardization of prompt templates, alignment of questions with instructional objectives, and format balancing to facilitate controlled comparisons across task types.

This revised dataset serves as the experimental substrate for probing how current LLMs perform in data-scarce, domain-specific scientific tasks. It enables both accuracy-based and semantic evaluations, supporting a deeper understanding of model behavior in hydrology-specific applications such as context comprehension, domain adaptation, and generalization across varied question formats. Figure 1 illustrates the overall workflow of this study, beginning with data sources from hydrology textbooks and peer-reviewed research articles. Domain-specific sources were used to generate instructional QA data with GPT-4o-mini.

This dataset was used to fine-tune various language models, and model performance was evaluated using accuracy and cosine similarity metrics. Using GPT-4o-mini and a series of carefully constructed prompts, we generated question–answer pairs aligned with hydrological learning objectives. These QA pairs served as the basis for fine-tuning a diverse set of LLMs. The final phase involved evaluating the performance of the fine-tuned models using both accuracy-based metrics (for multiple choice and true/false) and semantic similarity measures (for open-ended and fill-in-the-blank tasks).



Figure 1. Overview of the HydroLLM experiment pipeline.

To evaluate the effectiveness of fine-tuning on our hydrology dataset, we selected a diverse suite of language models varying in size and architecture, including [e.g., "DeepSeek R1 Distill Qwen 32B, 14B, 1.5B, DeepSeek R1 Distill Llama 8B, Llama-2-7b-chat-hf, and Qwen1.5-1.8B-Chat"]. Given the computational demands of fine-tuning these large-scale language models, all experiments were conducted on a dedicated high-performance computing infrastructure equipped with enterprise-grade GPUs (2 x NVIDIA H100 NVL 94 GB, 188GB total vRAM via NVLink). This setup ensured sufficient memory capacity and processing power to handle the iterative training processes required for our multi-model comparison study.

Hyperparameter optimization strategies varied across models based on their training behavior on our hydrology dataset. The DeepSeek R1 Distill Qwen 1.5B and 14B, DeepSeek R1 Distill Llama 8B, Llama-2-7B-chat-hf and Qwen1.5-1.8B-Chat models demonstrated stable training

dynamics without overfitting, enabling us to conduct hyperparameter tuning to identify optimal configurations for these architectures. In contrast, the larger 32B model exhibited severe overfitting tendencies on the specialized hydrology dataset, necessitating early stopping and preventing meaningful hyperparameter optimization. This differential behavior across model sizes guided our decision to focus optimization efforts on the 1.5B and 14B and Llama variants within the DeepSeek R1 Distill models, which showed capacity for generalization while maintaining sufficient model complexity for the domain-specific task.

2.3. Experiments

The experiments in this study were conducted as a diagnostic exploration to identify which existing language model architectures and fine-tuning strategies would be most appropriate for building HydroLLM. Rather than aiming to establish performance benchmarks, our goal was to empirically evaluate how different model sizes and instruction-tuned configurations behave under hydrology-specific fine-tuning conditions, particularly with a relatively small, curated dataset.

We began by experimenting with larger-scale models from the DeepSeek-R1-Distill family, including the 32B variant from the Qwen architecture. The 32B model exhibited severe overfitting to our 8,800-sample hydrology QA dataset, evidenced by dramatic divergence between training and validation loss curves even under conservative learning rate schedules and LoRA regularization. We attribute this behavior to the fundamental mismatch between the model's massive parameter capacity and our limited domain-specific supervision signals.

In contrast, smaller variants from the DeepSeek-R1-Distill family demonstrated stable training dynamics without overfitting tendencies. We systematically evaluated three base model architectures: the Qwen 1.5B and 14B variants, and the Llama 8B variant. These models enabled comprehensive hyperparameter optimization across learning rates, LoRA configurations, and regularization parameters.

Beyond exploring model size and architecture effects, we investigated whether instruction-tuning could improve performance on our structured QA tasks. Given that our hydrology dataset incorporates structured prompts requiring specific response formats (multiple choice, true/false, fill-in-the-blank, and open-ended), we hypothesized that instruction-tuned models might demonstrate superior performance due to their pre-training on instruction-following tasks. To test this hypothesis, we fine-tuned several instruction-tuned models—including Meta's Llama-2-7b-chat-hf and Qwen's Qwen1.5-1.8B-Chat—under identical dataset and training conditions as our base model experiments.

These models, pre-trained with instruction-following objectives, provided a useful contrast to DeepSeek's distilled variants and allowed us to assess whether prior exposure to instructional formatting would enhance domain adaptation in hydrology-specific tasks. All experiments utilized consistent training infrastructure and evaluation protocols to ensure fair comparison across model architectures. We applied LoRA fine-tuning to all models to maintain methodological consistency. Detailed overfitting analysis for the 32B model, including loss curve trajectories, is presented in

Section 3.1, while comprehensive performance comparisons across all tested models are provided in Section 3.2.

2.4. Evaluation

The evaluation of our fine-tuning experiments was carried out through a multi-layered framework aimed at diagnosing overfitting, assessing instructional alignment, and measuring performance across diverse QA formats using the HydroLLM-Benchmark (Kizilkaya et al., 2025). The primary goal was not to benchmark model performance in the conventional leaderboard sense, but rather to identify viable paths toward building a robust hydrology-specific LLM. Accordingly, our evaluation strategy combined training diagnostics, classification metrics, and semantic similarity scoring to gain nuanced insight into model behavior.

At the core of our initial evaluation, we closely monitored training loss curves and validation performance to detect overfitting. This step was particularly critical in our first set of experiments using the DeepSeek-R1-Distill-Qwen models (32B, 14B and 1.5B), where the larger models quickly demonstrated signs of overfitting despite standard regularization. In contrast, the 1.5B and 14B variants did not exhibit the same loss divergence. Once training stability was established, we turned to comprehensive performance evaluation across question formats. Beyond loss diagnostics, we employed task-specific evaluation metrics based on the nature of the QA format. For multiple choice and true/false questions, we computed simple classification accuracy by comparing the predicted label to the reference answer. These formats provide clear-cut correctness signals and serve as a baseline for instruction adherence.

For open-ended and fill-in-the-blank tasks, where multiple semantically valid completions may exist, we used cosine similarity between the model-generated answer and the reference answer. Embeddings were computed using a Sentence Transformers model (sentence-transformers/all-MiniLM-L6-v2), selected for its balance of computational efficiency and robust semantic representation capabilities across scientific domains. This approach enabled a more flexible evaluation of answer quality, especially in contexts where hydrological terminology or phrasing may vary. This evaluation framework allowed us to observe differences in how models performed across formats, instruction types, and fine-tuning regimes. These findings inform not only the selection of candidate architectures for HydroLLM, but also provide concrete signals about which model behaviors require targeted improvement in future iterations.

3. Results

The results of our experiments provide insights into how different language models perform under fine-tuning for hydrology-specific tasks. Rather than aiming to optimize for benchmark scores, our focus was on characterizing model behavior across different models and identifying architectures best suited for domain adaptation in data-limited settings.

3.1. Overfitting Behavior Across Model Scales

Our first series of experiments revealed significant differences in overfitting tendencies across model sizes. Despite adjustments to batch size, learning rate, and dropout, the model consistently failed to retain generalization, the 32B model demonstrated particularly severe overfitting behavior across multiple experimental configurations. In our initial experiment, training loss dropped precipitously from ~5.5 to near-zero within approximately 200 steps, while validation loss not only stagnated but actually increased from 6.53 to 6.74, creating a dramatic divergence indicative of complete memorization (Figure A.1).

Recognizing these clear signs of overfitting, we conducted a second experiment with substantially stronger regularization: increased dropout (0.05 → 0.1), reduced learning rate ($2e^{-4}$ → $5e^{-6}$), and enhanced weight decay (0.01 → 0.05). However, the training loss exhibited an identical rapid collapse pattern, dropping from ~5.5 toward zero within the first 50 steps. We implemented aggressive early stopping at this point to prevent computational waste and further degradation. The consistency of this behavior across different hyperparameter configurations reinforced our conclusion that the fundamental issue was the severe mismatch between model capacity (32B parameters) and dataset size (~8.8k examples), leading to inevitable memorization rather than generalizable learning.

3.2. Instruction-Tuned Model Performance

After fine-tuning, instruction-tuned models demonstrated competitive but generally inferior performance compared to the best-performing standard pre-trained models. The Llama2 7B Instruct model achieved solid results with 85.5% MCQ accuracy on book questions and 92.5% on articles, paired with robust true/false performance of 80.8% and 79.4%, respectively. The Qwen 1.5 1.8B Instruct model showed similar patterns, achieving 80.7% MCQ accuracy on book questions and 90.5% on articles, with consistent true/false performance at 69.7% and 76.4%.

Figure 2 shows that both instruction-tuned models outperformed the fine-tuned 1.5B Qwen model across most metrics, suggesting that instruction pre-training provides benefits for smaller model architectures. The average performance scores clearly demonstrate this hierarchy: Llama-2-7B-chat-hf achieved 70.5%, Qwen1.5-1.8B-Chat reached 68.9%, both substantially exceeding the DeepSeek-R1-Distill-Qwen-1.5B baseline of 54.4%. However, neither instruction-tuned model approached the performance levels of the top-performing fine-tuned DeepSeek models, with the leading DeepSeek-R1-Distill-Llama-8B achieving 75.7% and DeepSeek-R1-Distill-Qwen-14B reaching 71.1%. Despite being pretrained to follow instructions, these models exhibited limited adaptation to hydrology-specific concepts, particularly in fill-in-the-blank tasks that required precise terminology completion rather than general instruction-following.

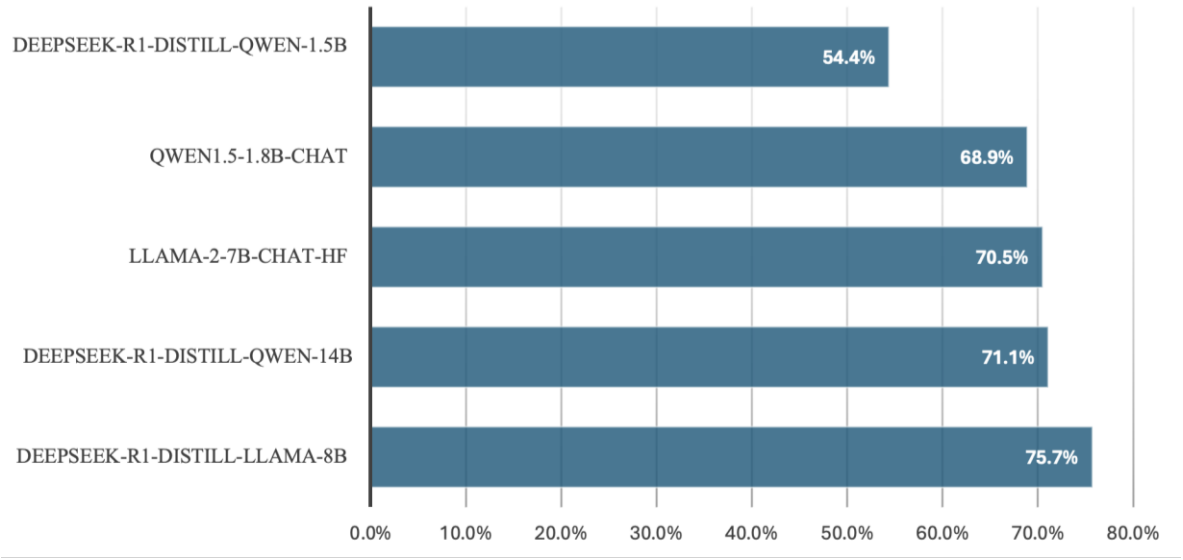


Figure 2. Overall model performance ranking based on average scores across all tasks.

3.3. Task-Specific Performance Analysis

Fill-in-the-blank (FITB) tasks emerged as the most challenging evaluation metric across all models. Among the models that demonstrated meaningful improvement with fine-tuning, the base versions struggled significantly with terminology completion, with performance ranging from 16.70% to 31.80% across different architectures and content sources (Figure 3). These three models—DeepSeek-R1-Distill-Llama-8B, Llama-2-7B-Chat, and Qwen1.5-1.8B-Chat—were selected for fine-tuning analysis based on their potential for improvement and architectural diversity.

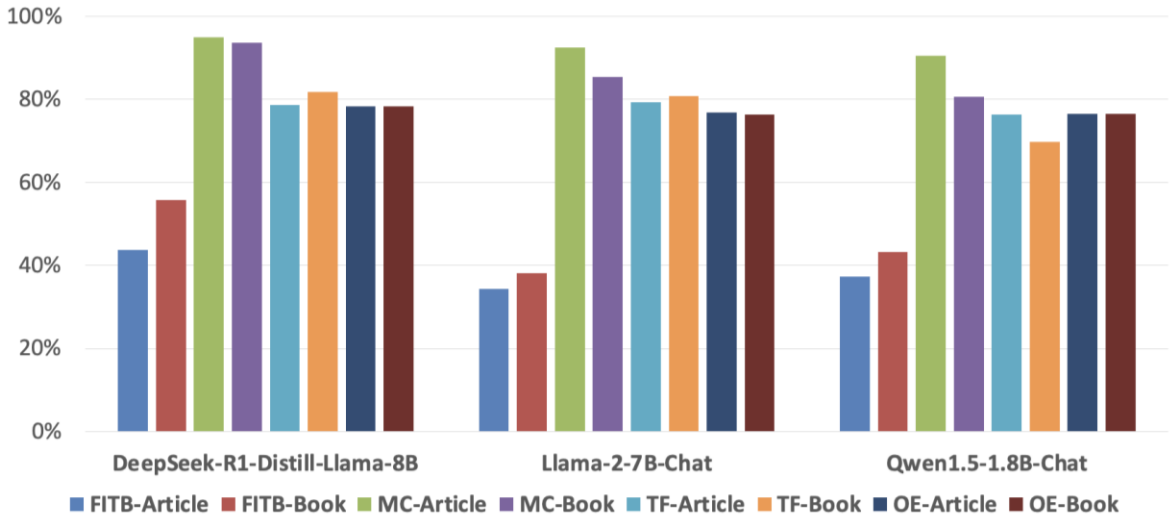


Figure 3. Fine-tuned Model Performance Across Question Types and Content Sources

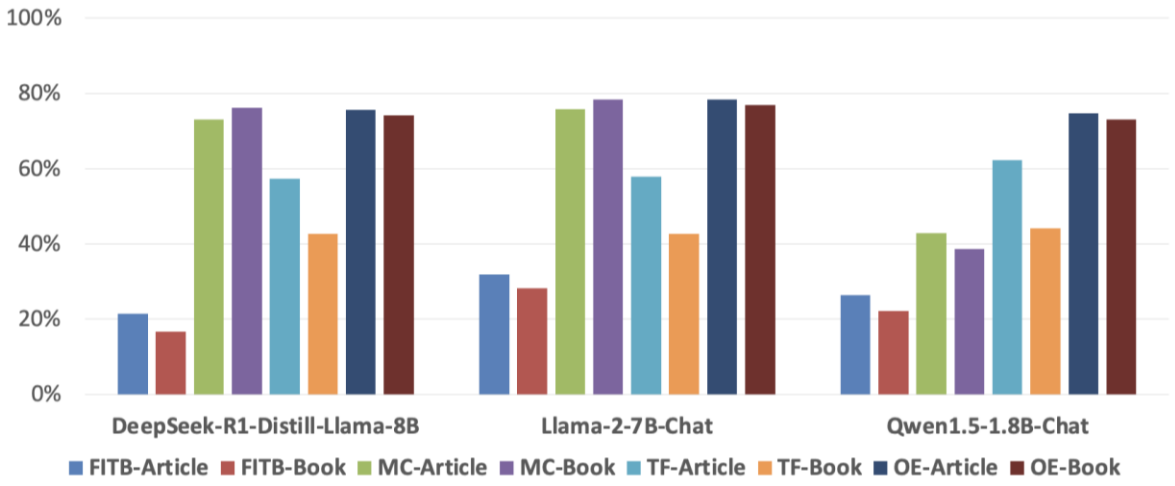


Figure 4. Base Model Performance Across Question Types and Content Sources

Fine-tuning transformed FITB capabilities substantially for these responsive models (Figure 4). The DeepSeek-R1-Distill-Llama-8B model achieved 55.7% accuracy on book questions and 43.7% on article questions, compared to its base performance of 16.7% and 21.4% respectively. Llama-2-7B-Chat reached 38.1% on book questions and 34.3% on article questions, while Qwen1.5-1.8B-Chat attained 43.2% and 37.3% respectively. While base models struggled with terminology precision, fine-tuning successfully enhanced their ability to complete domain-specific vocabulary across all tested architectures.

The selected models revealed distinct architectural responses to fine-tuning. The DeepSeek-R1-Distill-Llama-8B model showed particularly strong performance on book-derived FITB questions (55.7%) while maintaining solid article performance (43.7%). The Qwen1.5-1.8B model demonstrated more balanced performance across content sources, achieving 43.2% on book questions and 37.3% on article questions. Llama-2-7B-Chat showed consistent but more modest improvements, reaching 38.1% and 34.3% for book and article questions respectively. These differential responses underscore the importance of architectural consideration in domain-specific fine-tuning applications.

Multiple choice questions have demonstrated consistently high performance across these fine-tuning-responsive models. Base models have achieved strong accuracy, ranging from 38.6% to 78.4% depending on content source and model architecture (Figure 3). Fine-tuned versions showed additional gains, with all models achieving above 80.7% accuracy on book questions and most exceeding 90.5% on article questions (Figure 4). The strong baseline performance and consistent improvements across architectures suggest that multiple choice formats effectively leverage existing model capabilities while benefiting from domain-specific training.

True/false and open-ended questions showed moderate but consistent improvements across the improvement-responsive model subset. Base model true/false performance ranged from 42.7% to 62.2%, with fine-tuned variants achieving 69.7% to 81.8% across different content sources. Open-ended performance followed similar patterns, with base models ranging from 73.0% to 78.4% and fine-tuned versions reaching 76.3% to 78.4%. The consistent improvement patterns across these

three architectures validate their selection as representative cases for understanding fine-tuning effectiveness, while the smaller performance gaps compared to FITB tasks confirm that precise terminology completion remains the primary differentiator in domain-specific language model adaptation.

3.4. Overall Model Performance Rankings

Following comprehensive evaluation across all four question types and both data sources, clear performance hierarchies emerged among the tested architectures. The DeepSeek R1 Distill Llama 8B fine-tuned model emerged as the clear top performer across most metrics (Table 1). On book-derived questions, it achieved 93.7% accuracy on multiple choice questions and 81.8% on true/false questions. Performance on article-derived questions was even stronger, reaching 95.0% MCQ accuracy, though true/false performance dropped slightly to 78.6%. Notably, this model also demonstrated superior performance on fill-in-the-blank tasks, achieving cosine similarities of 0.557 and 0.437 for book and article questions respectively—substantially outperforming all other tested models on this challenging task type.

The DeepSeek R1 Distill Qwen 14B model showed excellent performance on structured question formats, achieving the highest individual scores on book-derived questions with 96.1% MCQ accuracy and 88.0% true/false accuracy. However, this model struggled significantly with fill-in-the-blank tasks, achieving cosine similarities of only 0.285 and 0.230 for book and article questions respectively. Performance on article-derived structured questions remained strong at 95.8% MCQ and 81.7% true/false accuracy.

Contrary to expectations based on training stability, the DeepSeek R1 Distill Qwen 1.5B model demonstrated the weakest overall performance despite successfully avoiding overfitting. MCQ accuracy reached only 75.4% on book questions and 79.6% on articles, while true/false performance was particularly poor at 54.6% and 42.2% respectively. Fill-in-the-blank tasks proved especially challenging, with cosine similarities below 0.21 across both data sources.

Table 1: Comprehensive Performance Results (%) Across All Models for Multiple-Choice (MC), True/False (TF), Fill-in-the-Blanks (FITB), and Open-Ended (OE) questions.

Models	TextBook				Article				Avg
	Accuracy		cos(θ)		Accuracy		cos(θ)		
	MC	TF	FITB	OE	MC	TF	FITB	OE	
DS-R1-Distill-Llama-8B	93.7	81.8	55.7	78.4	95.0	78.6	43.7	78.4	**75.7**
DS-R1-Distill-Qwen-14B	96.1	88.0	28.4	78.9	95.8	81.7	22.9	77.3	**71.0**
Llama-2-7B-chat-hf	85.5	80.8	38.1	76.3	92.5	79.4	34.3	76.9	**70.5**
Qwen1.5-1.8B-Chat	80.7	69.7	43.2	76.6	90.5	76.4	37.3	76.5	**68.9**
DS-R1-Distill-Qwen-1.5B	75.4	54.6	20.9	70.3	79.6	42.2	19.7	72.2	**54.4**

4. Discussions

Our diagnostic exploration of language model architectures for hydrology-specific fine-tuning reveals several counterintuitive findings that challenge conventional assumptions about model scaling and domain adaptation. Rather than confirming that larger models necessarily perform better, our experiments expose fundamental limitations in current approaches to specialized scientific language modeling. These findings have important implications not only for HydroLLM development but for the broader challenge of adapting large language models to data-limited scientific domains.

The severe overfitting observed in larger models highlights a critical challenge in domain-specific fine-tuning: when model parameter counts vastly outscale the number of supervision signals, even advanced optimization techniques struggle to prevent memorization. This suggests that the conventional "bigger is better" paradigm from general-purpose language modeling may not directly transfer to specialized domains with limited training data. Instead, our findings point toward the importance of finding an optimal capacity-alignment balance where models are sufficiently expressive for the domain complexity without being prone to memorization.

The consistently poor performance across all models on fill-in-the-blank tasks reveals a deeper limitation in current language modeling paradigms. Unlike multiple-choice or open-ended formats, FITB tasks require precise lexical selection and syntactic control, demanding both domain knowledge and exact terminology completion. Even proprietary models like GPT-4o-mini and o3-mini have previously exhibited this weakness (Kizilkaya et al., 2025), suggesting that this challenge appears to persist even in state-of-the-art models and represents an inherent limitation in current transformer architectures for tasks requiring precise, context-sensitive vocabulary completion rather than general language generation.

Our results with instruction-tuned models reveal an important boundary condition: while instruction pre-training provides general benefits for task formatting and response structure, it does not automatically translate to superior domain-specific performance. This suggests that instruction-following capabilities and domain expertise may require different types of training signals and optimization strategies. The competitive but ultimately inferior performance of instruction-tuned models indicates that domain specialization may require more targeted approaches than relying solely on general instruction-following abilities.

The superior performance of the 8B Llama variant compared to the larger 14B Qwen variant on certain tasks suggests that architectural differences may be as important as, if not more important than, parameter count for domain-specific applications. This finding challenges the assumption that larger models within the same family will necessarily perform better and highlights the need for systematic architectural exploration in specialized domains.

While our curated dataset represents a high-quality collection of hydrology-specific QA pairs, its scale remains modest compared to typical LLM training regimes. This raises important questions about the relative importance of data quality versus quantity in domain adaptation. Our results suggest that even high-quality, domain-relevant data may be insufficient if the volume does

not match the model's capacity, pointing toward the need for either more extensive data collection or more parameter-efficient approaches to domain specialization.

These findings have broader implications for developing language models in scientific domains, where high-quality training data is often scarce and expensive to generate. The challenges we observed suggest that successful scientific domain models may require fundamentally different approaches than general-purpose models, including specialized architectures, novel training objectives, or hybrid approaches that combine domain-specific fine-tuning with broader scientific knowledge.

4.1. Limitations

Despite the strengths and novel contributions of this study, several limitations should be acknowledged. First, the curated dataset, while comprehensive within the context of hydrology, remains relatively modest in size compared to the data volumes typically used for LLM training, which may constrain the model's generalizability and robustness. The dataset is also limited to English-language sources and does not incorporate multimodal data, such as hydrological diagrams, time-series data, or remote sensing imagery, which are increasingly important in hydrological research and practice.

Additionally, our evaluation relies on automated semantic similarity metrics and task-specific accuracies, which, while informative, may not fully capture deeper aspects of scientific reasoning or nuanced domain expertise. The possibility of subtle data leakage or overlapping with pretraining corpora in open-source models, especially when using widely available research articles, cannot be completely excluded. Finally, although overfitting diagnostics were carefully employed, the rapid advancement of both model architectures and training algorithms may yield different trends or optimal configurations in future experimentation. These limitations point to opportunities for subsequent research to expand dataset diversity, include multimodal and multilingual evaluation, and develop more exhaustive benchmarks for domain-specific scientific reasoning.

5. Conclusion

This work represents a crucial step toward the development of HydroLLM through a systematic exploration of model architectures and fine-tuning approaches for hydrology-specific tasks. Our experiments demonstrate that building effective domain-specialized language models requires careful consideration of the relationship between model capacity, dataset size, and task complexity. The finding that the 8B DeepSeek Llama model outperformed both larger and smaller variants challenges conventional scaling assumptions and provides concrete guidance for future model selection in scientific domains. Our results establish several key principles for domain-specific language model development: the importance of matching model capacity to available training data, the particular challenges posed by precise terminology completion tasks, and the limitations of instruction-tuning alone for achieving domain expertise. These insights provide a foundation for the continued development of HydroLLM and offer valuable lessons for the broader scientific machine learning community working on specialized domain adaptation.

Building robust domain-specialized models like HydroLLM requires moving beyond simple model scaling toward more nuanced approaches that consider task complexity, data characteristics, and architectural constraints. Several promising research directions emerge from our findings that warrant systematic investigation. Our study suggests several pathways for advancing HydroLLM through dataset enhancement, including expanding the current 8,800 QA pairs to include greater representational diversity across hydrological subdisciplines such as groundwater hydrology, urban drainage, ecohydrology, and hydrogeochemistry. Additionally, incorporating multimodal data such as hydrological diagrams, time series plots, and satellite imagery could enable more comprehensive reasoning capabilities, while synthetic data generation techniques specifically designed for hydrology could help address the fundamental data scarcity challenge while maintaining domain fidelity.

Future work should explore multi-stage training strategies that combine pretraining, instruction tuning, and domain-specific alignment in optimized sequences. Parameter-efficient training methods beyond LoRA, such as prefix tuning, adapters, and mixture-of-experts architectures, may offer better capacity-efficiency trade-offs for scientific domains. The development of curriculum learning approaches that progressively introduce concepts from basic hydrology to advanced applications could improve knowledge transfer and retention. The superior performance of certain architectures over others suggests opportunities for developing specialized model designs tailored to scientific reasoning, including hybrid architectures that combine transformer-based language modeling with physics-informed neural networks or graph neural networks to better capture the complex relationships inherent in hydrological systems.

Our findings highlight the need for more sophisticated evaluation approaches that better capture domain-specific competencies. Future work should develop evaluation benchmarks that assess not only factual accuracy but also scientific reasoning quality, uncertainty quantification, and the ability to identify and correct misconceptions. Practical deployment of HydroLLM requires integration with existing hydrological modeling tools, databases, and decision-support systems, focusing on creating APIs and interfaces that allow interaction with popular hydrological software packages like SWAT, MODFLOW, and HEC-RAS. The development of uncertainty-aware response generation and the ability to provide confidence estimates would be crucial for real-world scientific applications.

The methodological insights from this work extend beyond hydrology to other data-limited scientific domains. Future research should investigate the transferability of our findings to fields such as ecology, geology, atmospheric science, and environmental engineering, with cross-domain studies revealing universal principles for scientific domain adaptation while identifying field-specific requirements that necessitate specialized approaches. As interest in scientific language models continues to grow, the development of domain-aware design principles—encompassing both data curation and model architecture—will be essential to ensure that language models can truly support specialized scientific fields like hydrology in addressing the complex water challenges facing our world.

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Glossary

- **AGI (Artificial General Intelligence)**: A form of artificial intelligence characterized by flexible, human-like problem-solving abilities across a wide range of tasks, as opposed to narrow, task-specific AI.
- **Cosine Similarity**: A metric used to assess the similarity between two non-zero vectors by measuring the cosine of the angle between them. In this study, it is used to evaluate the semantic similarity between model-generated and reference answers.
- **DeepSeek R1 Distill (DS-R1-Distill)**: A family of open-source large language models that have undergone distillation—a process of compressing larger models into smaller, more efficient ones—based on prominent architectures like Qwen and Llama.
- **Domain-Specific Large Language Model (LLM)**: A large neural language model that is trained or fine-tuned to handle specialized vocabulary, concepts, and reasoning tasks within a particular scientific field, such as hydrology.
- **Embeddings**: Numerical representations of text (words, sentences, or phrases) in a high-dimensional vector space, enabling similarity and semantic analysis.
- **FITB (Fill-in-the-Blank)**: An instructional question format where a key concept or term is omitted from a sentence, requiring the respondent to supply the most contextually appropriate word or phrase.
- **Generalization**: The capacity of a model to perform accurately on new, unseen data that was not included in its training set.
- **GPT-4o-mini**: A smaller, computationally efficient variant of the GPT-4 large language model by OpenAI, used in this study for generating domain-aligned question–answer data.
- **Instruction-Tuned Model**: A language model that has undergone additional training to better follow human-written prompts and instructions, often improving performance on structured or task-oriented queries.
- **LoRA (Low-Rank Adaptation)**: A parameter-efficient fine-tuning method that updates a low-rank subset of a model's parameters, enabling rapid specialization to new domains with less risk of overfitting.
- **MCQ (Multiple-Choice Question)**: A common question format offering discrete answer options, from which the correct response must be selected.
- **Open-Ended (OE)**: A question format that prompts the respondent to generate a freeform, natural language response without predefined options.
- **Overfitting**: A modeling issue where a machine learning algorithm learns patterns too specific to the training set, resulting in poor generalization to new data.

- **Qwen**: An open-source large language model architecture developed by Alibaba, used as one of the baseline architectures in this study.
- **Semantic Similarity**: A measure of how closely the meaning of two pieces of text align, regardless of the exact wording used.
- **True/False (TF)**: An instructional format where respondents judge the veracity of a given statement.

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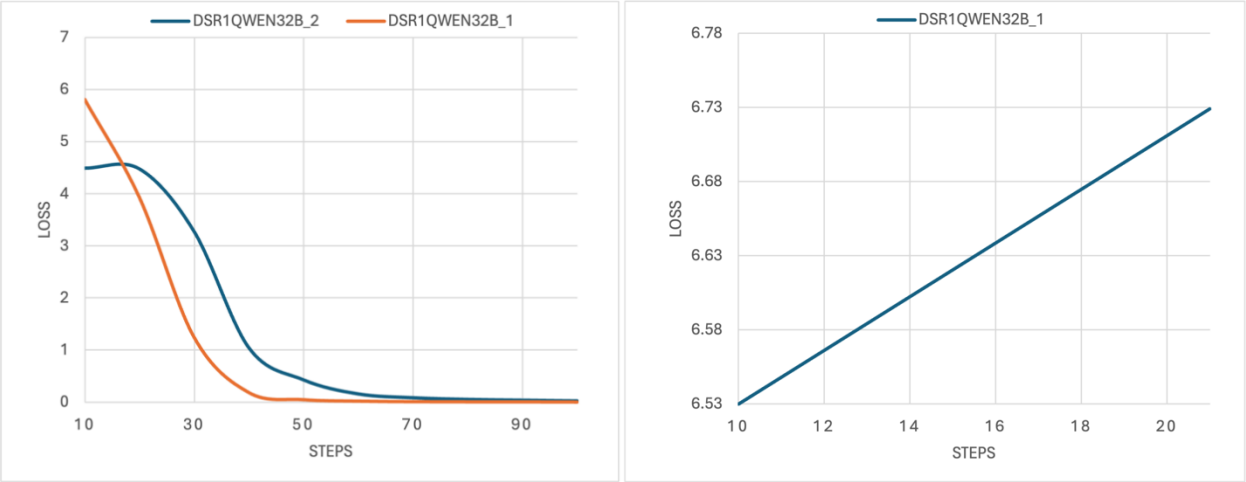
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Appendix



(a) (b)

Figure A1. Training and validation loss curves for DeepSeek-R1-Distill-Qwen-32B experiments. **(a) Experiment 1** demonstrates severe overfitting with training loss dropping to near-zero while validation loss increases. **(b) Experiment 2** was terminated at step ~50 upon detecting the same rapid training loss collapse, before validation evaluation was triggered.