Domain-Specific Embedding Models for Hydrology and Environmental Sciences: Enhancing Semantic Retrieval and Question Answering in RAG Pipelines

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Abstract

Large Language Models (LLMs) have shown strong performance across natural language processing tasks, yet their general-purpose embeddings often fall short in domains with specialized terminology and complex syntax, such as hydrology and environmental science. This study introduces HydroEmbed, a suite of open-source sentence embedding models fine-tuned for four QA formats: multiple-choice (MCQ), true/false (TF), fill-in-the-blank (FITB), and open-ended questions. Models were trained on the HydroLLM Benchmark, a domain-aligned dataset combining textbook and scientific article content. Fine-tuning strategies included MultipleNegativesRankingLoss, CosineSimilarityLoss, and TripletLoss, selected to match each task's semantic structure. Evaluation was conducted on a held-out set of 400 textbook-derived QA pairs, using top-k similarity-based context retrieval and GPT-4o-mini for answer generation. Results show that the fine-tuned models match or exceed performance of strong proprietary and open-source baselines, particularly in FITB and open-ended tasks, where domain alignment significantly improves semantic precision. The MCQ/TF model also achieved competitive accuracy. These findings highlight the value of task- and domain-specific embedding models for building robust retrieval-augmented generation (RAG) pipelines and intelligent QA systems in scientific domains. This work represents a foundational step toward HydroLLM, a domain-specialized language model ecosystem for environmental sciences.

Keywords: Domain-Specific Embeddings, Fine-Tuning, HydroLLM, Large Language Models (LLM), Retrieval-Augmented Generation (RAG), Semantic Retrieval

Highlights

- Introduced HydroEmbed, a suite of domain-specific sentence embedding models for hydrology.
- Fine-tuned models support MCQ, TF, FITB, & Open-Ended QA formats with task-aligned loss functions.
- Trained on the HydroLLM Benchmark dataset of textbooks and scientific articles.
- Outperform general-purpose and open-source baselines on domain-specific retrieval.
- A foundational step toward HydroLLM, a specialized language model for hydrological applications.

1. Introduction

Large Language Models (LLMs), such as GPT-4 and Claude, have demonstrated state-of-the-art performance across a wide array of natural language processing (NLP) tasks, including reasoning, summarization, and question answering. Their strengths lie in generalization capabilities, achieved through training on vast corpora and advanced architectural designs. These models excel in both associative “System 1” thinking and more deliberate “System 2” reasoning, particularly when augmented with techniques such as Chain-of-Thought prompting (Plaat et al., 2024).

In educational and scientific contexts, LLMs have achieved notable results, for instance, GPT-4’s performance in professional exams in biology and environmental science underscores its ability to integrate domain knowledge and execute complex reasoning (Gong et al., 2023; Pursnani et al., 2023). Their effectiveness in zero-shot question answering and summarization further solidifies their role in modern NLP pipelines (Espejel et al., 2023; Matarazzo & Torlone, 2025; Yadav, 2024). Building upon these successes, recent investigations have demonstrated the applicability of smart assistants in domain-specific scientific and environmental applications, such as hydrology, where they enable advanced analysis and interpretation of complex data (Kadiyala et al., 2024a), and in public health contexts via semantic web frameworks for automated smart assistants (Sermet & Demir, 2021). Recent advances also highlight the promise of LLMs in educational applications, such as conversational AI-enabled assistants and intelligent learning systems, which personalize academic support and facilitate domain-specific knowledge acquisition across disciplines including environmental sciences (Shrestha et al., 2025; Sajja et al., 2025a; 2025b).

Despite these advances, the embedding spaces of general-purpose LLMs often struggle to encode the specialized terminology and conceptual nuances found in scientific literature. This limitation is particularly acute in domains like chemistry, medicine, and environmental science, where complex syntax and domain-specific vocabulary are prevalent (Leivada et al., 2023; Dubey & Kohli, 2023). Emerging approaches seek to address these shortcomings. For example, Tag-LLM introduces continuous vector tags to condition LLMs for domain-specific reasoning (Shen et al., 2024), while methods like vector embedding augmentation and continual fine-tuning on specialized corpora have shown promise in adapting models for technical fields (Wolfrath et al., 2024; Hatakeyama-Sato et al., 2023).

Complementing these methods, new educational embedding models have been fine-tuned specifically for academic content retrieval, demonstrating superior performance in question matching, course document parsing, and retrieval-augmented generation (Sajja et al., 2025c). These enhancements support the development of chatbots and semantic search tools capable of handling the nuanced structures and synonymy present in course materials in academic and professional training settings (Pursnani et al., 2025).

Hydrology and environmental science exemplify these challenges. As data-rich, interdisciplinary fields, they incorporate physical process modeling, climatic variability, and human-environmental interactions. Hydrological systems are shaped by complex interdependencies across meteorology, geology, and land use, requiring precise language to describe phenomena such as soil infiltration, runoff dynamics, evapotranspiration, and groundwater flow (Salas et al., 2013; Vogel et al., 2015; Shapiro & Day-Lewis, 2022).

In this context, domain ontologies offer a promising avenue for improving both the performance and interpretability of embedding models in hydrology and environmental sciences. Ontologies provide structured semantic relationships, such as is-a, part-of, and has-property, that enrich the embedding space with explicit, human-curated knowledge. This allows models to better capture domain-specific nuance and achieve superior accuracy in classification, similarity computation, and scientific reasoning tasks (Chen et al., 2020; Benarab et al., 2023; Ronzano & Nanavati, 2024).

Embedding methods that incorporate ontological structure, particularly when combined with lexical metadata, outperform standard embeddings on tasks like class membership prediction, function annotation, and similarity evaluation (Chen et al., 2024; Ibtehaz et al., 2023; Kulmanov et al., 2020). Moreover, models fine-tuned using ontology-guided supervision show stronger domain alignment and better generalization across related scientific tasks, especially when multiple, aligned ontologies are used as priors (Wang et al., 2023; Ronzano & Nanavati, 2024; Chen et al., 2024).

Beyond performance gains, ontologies substantially enhance interpretability. Because ontology-based embeddings map to structured, human-understandable concepts, they allow users to trace model outputs to recognizable domain knowledge (Cheong et al., 2023; Zhang et al., 2024). By grouping embedding dimensions by ontological categories, it becomes possible to generate domain-level explanations, increasing transparency and trust in model predictions (Zhang et al., 2024; Jia et al., 2025). Additionally, the integration of attention mechanisms with ontological metadata enables interpretive insights into which concepts or relationships drive specific decisions (Cheong et al., 2023; Jia et al., 2025).

Moreover, hydrology spans technical subfields such as ecohydrology, hydrogeochemistry, and sociohydrology, all of which contribute to specialized and evolving scientific vocabulary and ontologies (Sermet and Demir, 2019; Younger et al., 2002; Baydaroglu et al., 2022). The structural complexity of texts in this domain, including layered clauses, compound sentences, and embedded rhetorical devices, further limits the effectiveness of general-purpose embeddings (Saeeaw & Tangkiengsirisin, 2014; Zhang et al., 2023; Yan et al., 2022). A bibliometric review of LLM adoption in environmental sciences underscores the domain's growing reliance on AI for modeling, forecasting, and monitoring, while identifying challenges around data transparency, ethical deployment, and computational scalability (Sajja et al., 2025d).

General-purpose embedding models like BERT and OpenAI's proprietary embeddings show decreased performance when applied to tasks involving specialized technical or legal text. This is due to their limited exposure to domain-specific linguistic patterns during pretraining, which results in semantic drift, poor contextual interpretation, and reduced classification accuracy in downstream tasks (Hua et al., 2022; Boukkouri et al., 2019; Tang & Yang, 2024; Mukherjee & Hellendoorn, 2023).

Domain-specific embeddings, such as ClinicalBERT and BioBERT, address these limitations by tailoring the representation space to the unique language structures of their target fields, thereby enhancing contextual precision and reducing issues like polysemy and homonymy (Braun et al., 2021; Yunianto et al., 2020; Rongali et al., 2020). These models have proven especially useful in capturing semantic nuance, establishing terminological relationships, and building more coherent knowledge bases in their respective disciplines (Eitan et al., 2023; Wang et al., 2023; Faber et al., 2008). Beyond academic and clinical contexts, AI-enhanced decision support systems have also been applied in complex environmental planning scenarios, such as flood mitigation or water quality strategy development, illustrating the power of role-based AI agents in multi-stakeholder simulation environments (Kadiyala et al., 2024b; Samuel et al., 2024).

However, deploying closed-source models like those offered by OpenAI presents additional challenges. These models operate as opaque systems, limiting interpretability, reproducibility, and ethical auditability. The black-box nature of closed models poses serious concerns in sensitive applications such as environmental risk assessment and policy making process (Manchanda et al., 2024; Zarlenga et al., 2022). Furthermore, closed models can create barriers to access and innovation, as their proprietary status hinders reproducibility and cross-institutional collaboration (Widder et al., 2024). Balancing adversarial robustness with explainability remains a key challenge in designing actionable and trustworthy AI systems (Krishna et al., 2024).

To address the limitations of general-purpose embeddings in technical domains, we introduce a set of domain-specific embedding models fine-tuned explicitly for hydrology and environmental sciences. Hydrology, with its reliance on specialized vocabulary, complex physical models, and context-rich terminology, presents unique challenges for standard NLP systems trained primarily on general-language corpora. The models developed in this work are optimized for semantic relevance and contextual accuracy, enabling integration into retrieval-augmented generation (RAG) pipelines, domain-specific question answering systems, and intelligent tools for environmental knowledge exploration. Training data is curated from the HydroLLM Benchmark dataset (Kizilkaya et al., 2025), which includes instructional content from both hydrology textbooks and peer-reviewed scientific articles.

We employ multiple fine-tuning methodologies, including MultipleNegativesRankingLoss (MNRL), CosineSimilarityLoss, and TripletLoss, to enhance both ranking behavior and semantic alignment. These strategies are adapted to the distinct characteristics of each QA format: multiple-choice (MCQ), true/false (TF), fill-in-the-blank (FITB), and Open-Ended questions. The resulting models are benchmarked against proprietary and open-source baselines across all formats, demonstrating clear advantages in contextual relevance, semantic similarity, and retrieval precision. Through this work, we contribute transparent, reusable, and domain-specific embedding models tailored for hydrology and environmental sciences, advancing the development of trustworthy, performant, and accessible AI systems for specialized scientific applications. This effort also serves as an early milestone toward the broader vision of HydroLLM: a comprehensive, domain-specific language model ecosystem for hydrology and environmental sciences.

2. Methodology

Given the linguistic complexity and domain-specific terminology of environmental texts, a modular training approach was adopted to address the unique requirements of different question formats. We begin by describing the structure and intent of each question-answering (QA) task, followed by a detailed overview of the dataset used for training and evaluation. Subsequent subsections cover corpus preprocessing, embedding and retrieval workflows, model architecture choices, fine-tuning strategies tailored to each QA type, and the training configuration used across experiments.

2.1. Task Overview

This study addresses four distinct QA formats that are commonly encountered in scientific education and technical assessment: MCQ, TF, FITB, and open-ended questions. These formats differ significantly in structure, answer style, and linguistic complexity, each posing unique challenges for NLP systems. The design of the embedding models in this study is therefore tailored to accommodate the semantic and contextual demands of each task type.

MCQ consists of a question stem followed by several predefined answer options, typically labeled A through D. To answer such questions, a model must accurately retrieve relevant information from the context and identify the correct option. In addition to basic fact retrieval, MCQs often require nuanced understanding to distinguish between closely related distractors, an ability that hinges on fine-grained semantic discrimination.

TF questions present a binary classification challenge, where the model must assess the truthfulness of a factual statement. These tasks often involve subtle semantic cues such as negation, numeric qualifiers, or domain-specific language that must be correctly interpreted in light of retrieved evidence. Despite their binary nature, TF questions demand high contextual precision, particularly in scientific domains where accuracy is critical.

FITB questions follow a cloze-style format, where key tokens have been intentionally removed from a sentence. The model's objective is to infer the missing word or phrase based on syntactic structure and surrounding semantic cues. FITB questions place strong emphasis on lexical alignment and localized phrase-level matching, making them especially useful for testing the embedding model's ability to encode fine-grained context.

Open-Ended questions require free form, unconstrained responses and often involve explanatory or descriptive language. These questions demand that the model synthesize information across multiple retrieved passages to construct coherent, contextually appropriate answers. Among all formats, open-ended questions are the most semantically rich and variable, requiring broad contextual reasoning and high representational flexibility from the embedding model.

To support reproducible evaluation, each question in the benchmark dataset is paired with a ground-truth answer. This enables objective comparison of predicted versus reference responses across formats. The inclusion of diverse QA types allows for a comprehensive analysis of model adaptability, retrieval precision, and semantic robustness. Table 1 provides representative examples of each question format to illustrate the structural and linguistic differences among them.

Table 1: Example Questions Categorized by Question Type

Category	**Natural Language Questions**
MCQ	What is a common issue when gauging flow in gravel-bed rivers? A) The water temperature fluctuates greatly, B) The riverbed profile changes frequently, C) There are too few measurement points
True/False	The hydraulic gradient is the slope of the water table in an aquifer.
Fill in the Blank	Flood frequency analysis is concerned with peak flows and normally records these separately to ___________ mean flows.
Open-Ended	What is the significance of using historical flow data in instream flow assessments?

2.2. Dataset and Benchmark

This study utilizes the HydroLLM Benchmark (Kizilkaya et al., 2025), a curated dataset developed to evaluate language models in the context of hydrology and environmental sciences. The benchmark is constructed to support both semantic retrieval and question answering by incorporating a diverse range of linguistic expressions and question types relevant to scientific and educational discourse. Its design reflects the need for evaluating models on real-world, domain-aligned tasks rather than relying solely on general-purpose QA datasets.

The dataset comprises two primary content sources. The first consists of textbook material, which offers structured, pedagogically organized knowledge ideal for foundational learning and context alignment. The second source includes peer-reviewed scientific articles that capture the domain-specific language, complexity, and variability of real-world scientific communication.

Together, these sources ensure a balance between accessibility and linguistic richness, allowing the trained models to generalize across both instructional and technical subdomains.

Four distinct QA formats are included in the dataset: MCQ, TF, FITB, and open-ended questions. Each format introduces different semantic and structural demands, requiring tailored model capabilities. Importantly, every QA pair is accompanied by a ground truth answer, enabling precise and objective evaluation of retrieval and reasoning performance across formats. Each question is also linked to a corresponding source document excerpt, supporting the retrieval tasks that precede answer generation in the RAG framework.

For evaluation purposes, a test set was constructed by randomly selecting 100 textbook-derived questions for each QA format, resulting in a balanced and format-diverse set of 400 test items. All evaluation questions were drawn exclusively from textbook content to ensure consistent and controlled context retrieval. This restriction was necessary because the article-derived questions are not tied to chunked or indexed source documents, making embedding-based retrieval infeasible for these examples under current benchmark constraints.

The remaining QA pairs, those not included in the test set, comprise the training corpus. This training data includes 2,169 open-ended QA examples, 1,120 FITB examples, and 2,542 MCQ and TF examples. For the FITB format, an additional 1,120 triplet instances were constructed using an anchor (the FITB question), a positive (correct answer), and a hard negative (plausible but incorrect answer) to facilitate contrastive training via TripletLoss. Although questions derived from research articles were excluded from the evaluation set, they were fully retained in the training set, adding valuable diversity in linguistic patterns and scientific terminology.

This configuration supports both controlled evaluation and domain-robust training. By relying on structured textbook content for testing and leveraging the broader domain variance of articles for training, the HydroLLM Benchmark enables comprehensive, reproducible benchmarking of domain-specific embedding models tailored to hydrology and environmental science.

2.3. Corpus Preprocessing and Embedding Workflow

To support effective semantic retrieval across diverse QA formats, the source documents in the HydroLLM Benchmark were preprocessed into uniform text segments using a fixed-length chunking strategy. Specifically, all textbook content was divided into approximately 300-character chunks, ensuring a balance between contextual completeness and embedding granularity. This chunk length was chosen to preserve sentence-level coherence while enabling dense vector indexing and efficient retrieval. Chunking was applied without overlapping windows to simplify memory usage and maintain clarity in source-reference alignment.

Once the corpus was chunked, sentence embeddings were generated for each segment using the same embedding model being evaluated (either baseline or fine-tuned). During inference, a test question is embedded into the same vector space. Cosine similarity is then computed between the question vector and all document chunk vectors, resulting in a ranked similarity list. This method enables the identification of semantically relevant content even when the surface phrasing of the source and question differ, an essential feature for domain-specific QA where terminology and syntax can vary considerably.

From the similarity-ranked results, the top three most similar chunks are retrieved to serve as contextual support for answering the question. We fixed $k = 3$ to control context length and isolate the contribution of the embedding model rather than variability in retrieval breadth. In preliminary trials, increasing $k$beyond 3 often introduced redundant or off-topic passages, adding noise that reduced answer quality. We acknowledge that cosine-based top-k retrieval can overweight lexical similarity; therefore, future work will explore adaptive-k thresholds, diversity-promoting methods such as Maximal Marginal Relevance (MMR), and cross-encoder reranking to improve semantic coverage.

For answer generation, we use GPT-4o-mini, a compact yet highly capable generative language model, to produce responses based on the retrieved context and the question prompt. GPT-4o-mini is invoked with a format-specific system instruction to align its generation behavior with the intended QA format, be it selecting from options, evaluating a truth value, inserting a missing term, or generating a free-text explanation. By decoupling the embedding model from the generative model, we isolate the performance of the embedding layer in the retrieval phase while leveraging GPT-4o-mini for consistent and high-quality language generation. GPT-4o mini is used as a fixed decoder across all experiments, ensuring that any performance difference arises from the embedding model's ability to retrieve relevant context rather than variation in the answer generator.

2.4. Model Architecture and Baseline

All embedding fine-tuned models developed and evaluated in this study are built upon the all-MiniLM-L6-v2 architecture, an open-source sentence embedding model from the Sentence-Transformers project (Reimers & Gurevych, 2019). This architecture was selected for its ideal balance between performance, efficiency, and accessibility. Despite its compact size, all-MiniLM-L6-v2 achieves competitive results on a wide range of semantic similarity and retrieval benchmarks, making it a practical foundation for domain-specific fine-tuning. Its lightweight design enables low-latency inference, which is critical for integration into real-time educational or environmental information systems. Furthermore, its open licensing and transparent architecture facilitate reproducibility, adaptability, and broader adoption within academic and open research communities.

To contextualize the performance of our domain-specific models, we benchmarked them against a mix of proprietary and open-source baselines widely used in natural language processing and RAG pipelines. Proprietary baselines include OpenAI's text-embedding-ada-002, known for its high utility in commercial applications, as well as the more recent text-embedding-3-small and text-embedding-3-large models, which offer improvements in semantic precision and efficiency. While these models provide strong performance, their closed-source nature limits transparency and interpretability, particularly important in scientific domains where auditability is essential.

On the open-source side, we compare our fine-tuned models with several representative baselines from the Sentence-Transformers library. These include the original all-MiniLM-L6-v2, the multi-qa-MiniLM-L6-cos-v1 model optimized for question answering tasks, msmarco-distilbert-base-v4 trained specifically for document-level retrieval, and nli-roberta-base-v2, which is aligned with natural language inference tasks and captures sentence-level semantic relationships.

2.5. Fine-Tuning Strategies

To adapt the base embedding architecture to the diverse structural and semantic demands of each QA format in the HydroLLM Benchmark, we implemented task-specific fine-tuning strategies. Each strategy was selected based on the linguistic structure and retrieval requirements of the question type, with the goal of optimizing semantic alignment and retrieval precision. All models were fine-tuned using variations of contrastive learning, leveraging ground truth answers and carefully constructed negative samples.

Multiple Choice & True/False: For MCQ and TF questions, where the task involves selecting the correct option from a finite set, we employed Multiple Negatives Ranking Loss (MNRL). This loss function is designed to encourage the model to bring semantically correct pairs, such as a question and its corresponding correct answer, closer together in the embedding space, while simultaneously pushing apart mismatched pairs.

During training, each batch was structured using an in-batch negative sampling approach, where every positive pair (question and correct answer) was implicitly paired with other batch items as negative examples. This method scales efficiently while providing strong contrastive supervision. The primary goal in this setup is to maximize the model's ability to distinguish between semantically close distractors, which are common in scientific MCQs and factual TF assertions.

Fill-in-the-Blank: The FITB format presents a unique challenge that demands both lexical precision and contextual coherence. To model this effectively, we used a dual-loss training setup combining TripletLoss and CosineSimilarityLoss. This configuration allows the model to simultaneously learn absolute semantic alignment and relative semantic distinction. For CosineSimilarityLoss, each training instance consisted of a (question, correct completion) pair, encouraging the model to embed semantically aligned text closely. For TripletLoss, we created structured training examples in the form of (anchor, positive, hard negative), where the anchor is the cloze-style question, the positive is the correct answer, and the negative is a plausible but incorrect filler sourced from another question. This contrastive approach promotes sensitivity to fine-grained phrase-level differences, essential for close tasks in domains with technical vocabulary and subtle terminology variation.

Open-Ended: Open-Ended questions require the model to support free-form, often multi-sentence answers. These tasks present the highest degree of semantic variability and require the embedding model to preserve descriptive nuance and conceptual fidelity. To support this, we used a hybrid loss strategy that combines Cosine Similarity Loss with MNRL. Cosine Similarity

Loss ensures that the model aligns semantically related question-answer pairs in the embedding space, even when the answer phrasing varies. Simultaneously, MNRL introduces contrastive pressure by treating other examples in the batch as negative samples, helping the model separate contextually irrelevant responses. This dual-objective configuration strikes a balance between semantic generalization and discriminative capability, both of which are critical for handling the open-ended, multi-faceted answers common in environmental and hydrological education.

2.6. Generalizability and Overfitting controls

To reduce the risk of overfitting and clarify generalization, we adopted the following controls. First, we enforced a strict instance-level split: no QA pair appearing in the training set appears in the held-out test set. Training supervision consists solely of (question, answer) pairs (and structured negatives where applicable), whereas evaluation retrieval operates over chunked textbook passages that the model does not observe during training. Accordingly, the model learns to align questions and answers at the representation level but must retrieve semantically relevant document chunks at inference time, decreasing the chance of rote memorization of evaluation content.

Second, we used conservative optimization and regularization, AdamW, a small learning rate, and warmup cosine scheduling, to support stable convergence and mitigate overfitting. Finally, we note a current limitation: the evaluation corpus is textbook-derived, while article-derived QA (present in training) was excluded from evaluation due to the lack of chunked, indexable article passages under current benchmark constraints. In future work, we will (i) perform leave-one-textbook-out evaluation to test cross-source generalization and (ii) reformat and index article content to enable an external-domain evaluation set consistent with our retrieval protocol.

2.7. Training Details

All models in this study were trained using the AdamW optimizer with a fixed learning rate of $2.e^{-5}$ and a weight decay of 0.01. A Warmup Cosine learning rate scheduler was employed across all configurations, with warmup steps comprising 10% of total training steps for the Open-Ended model and 15% for both FITB and MCQ/TF models. Additionally, Automatic Mixed Precision (AMP) was enabled in all training runs to enhance computational efficiency and reduce memory consumption without sacrificing numerical stability. For the Open-Ended model, training was conducted over 20 epochs. A batch size of 32 was used for cosine similarity-based training and 64 for contrastive ranking (MNRL). The smaller warmup proportion (10%) allowed for more gradual learning during the early epochs, which was particularly beneficial given the greater syntactic complexity and semantic depth of open-ended responses.

The FITB model was trained for 15 epochs, using a uniform batch size of 32 across both the TripletLoss and CosineSimilarityLoss objectives. A 15% warmup period was selected to ensure stable convergence, especially given the dual-loss configuration and the need to capture both structural and semantic precision. The MCQ/TF model was also trained for 20 epochs with a batch size of 32. A 15% warmup schedule was used to accommodate the sharper learning curves typically observed in classification-style tasks, where models must quickly learn to differentiate between closely related distractors.

To support deployment in resource-constrained environments, we also measured encoder-side efficiency for all HydroEmbed models. Each model contains 22.7M parameters (~86 MB on disk) and was evaluated on an NVIDIA RTX 3060 GPU. During encoding, peak memory usage was approximately 0.10 GB of VRAM. Single-sentence latency ranged from 4–6 ms (p50) and 5–6 ms (p95), while batch throughput (batch size = 32) ranged from 3,600 to 5,800 sentences per second, depending on the QA format. On CPU, single-query latency remained below 50 ms, confirming suitability for real-time or near-time applications. Importantly, all document embeddings in our RAG pipeline are precomputed offline, so online inference requires only (i) encoding a single query and (ii) performing a fast nearest-neighbor lookup over the embedding index (typically <1–2 ms). As a result, end-to-end per-query cost is dominated by a single encoder pass, making the HydroEmbed models lightweight enough for deployment in environmental monitoring tools and low-resource systems.

3. Results and Discussion

The results are analyzed across four QA formats, MCQ, TF, FITB, and Open-Ended, each representing distinct linguistic and semantic challenges. The evaluation metrics are tailored to each format, followed by a comparison of performance across proprietary, open-source, and domain-specific models. The discussion contextualizes these findings, highlighting the impact of task-specific training strategies, the limitations of general-purpose embeddings in specialized domains, and the implications for RAG and domain-specific QA pipelines.

3.1. Evaluation Metrics

The evaluation of model performance is tailored to the structure of each QA format. For MCQ and TF questions, accuracy is used as the primary metric. This involves a direct comparison between the model-generated answer and the ground truth label provided by the HydroLLM Benchmark dataset. An answer is considered correct only if it matches the expected choice or assertion exactly. This categorical evaluation provides a clear measure of precision in selecting the correct answer among a limited set of predefined options.

For FITB and Open-Ended questions, where valid answers may vary in phrasing but convey equivalent meanings, cosine similarity is used to evaluate semantic alignment between the model-generated response and the reference answer. Both the model output and the ground truth are converted into vector embeddings using the same encoder model, and their cosine similarity score is computed. This metric captures the degree of semantic overlap and provides a continuous measure of answer quality, which is more appropriate for tasks that involve natural language generation rather than classification.

3.2. Benchmarked Models

To evaluate the effectiveness of domain-specific fine-tuning, we benchmark our model against both proprietary and open-source embedding baselines commonly used for semantic similarity and retrieval tasks. The comparison includes models from OpenAI's text-embedding family as well as several popular open-source Sentence-Transformers models trained on general-purpose and QA-specific corpora.

The proprietary models include OpenAI's text-embedding-ada-002, a widely adopted general-purpose embedding model, and its successors, text-embedding-3-small and text-embedding-3-large, which offer improved performance and efficiency. These models serve as strong closed-source baselines, though they remain opaque in architecture and training data. Among the open-source baselines, we include all-MiniLM-L6-v2 for its efficiency and general-purpose performance, multi-qa-MiniLM-L6-cos-v1 for its optimization on QA tasks, msmarco-distilbert-base-v4 for retrieval-specific tuning on MS MARCO, and nli-roberta-base-v2 for alignment with natural language inference tasks.

Our proposed model is trained specifically in hydrology and environmental sciences using the HydroLLM Benchmark dataset. It incorporates tailored fine-tuning strategies for each question type (MCQ, TF, FITB, and Open-Ended) using a combination of Multiple Negatives Ranking Loss, Cosine Similarity Loss, and Triplet Loss. Unlike general-purpose models, it is optimized for semantic precision in domain-specific retrieval and QA tasks. This allows for more accurate alignment with the linguistic characteristics and scientific terminology of environmental content.

3.3. Performance Comparison

Table 3 presents the performance of the proposed fine-tuned models alongside widely used proprietary and open-source embedding baselines across three question formats: MCQ/TF, FITB, and Open-Ended. The evaluation was conducted using task-specific metrics, accuracy for MCQ/TF and cosine similarity for FITB and Open-Ended responses.

It is important to note that each fine-tuned model in this study was task-specific and was evaluated only on the QA format it was explicitly trained for. For example, the MCQ/TF model was not applied to FITB or Open-Ended tasks, and vice versa. This design choice ensures that performance metrics reflect a fair assessment of each model's capabilities within its intended context, without overextending them to unseen formats.

For MCQ/TF tasks, the fine-tuned model trained using MNRL achieved 93.5% accuracy, which is comparable to or slightly below top proprietary baselines such as text-embedding-3-large and text-embedding-3-small (both 95.5%) and ada-002 (95.0%). It matches or slightly outperforms open-source alternatives such as all-MiniLM-L6-v2 (93.0%) and msmarco-distilbert-base-v4 (93.0%).

Table 2: Overview of Evaluated Embedding Models

Category	Model Name	Description

Proprietary (Closed)	text-embedding-ada-002 (Greene et al., 2022)	General-purpose embedding model from OpenAI, optimized for cost-efficiency and widely used in commercial NLP tasks.
	text-embedding-3-small (OpenAI, 2024)	Lightweight model from OpenAI's latest series, designed to balance performance and inference cost for broad semantic retrieval tasks.
	text-embedding-3-large (OpenAI, 2024)	Flagship embedding model from OpenAI offering state-of-the-art performance in text similarity and semantic understanding across diverse domains.
Open Source	all-MiniLM-L6-v2 (Reimers& Gurevych, 2019)	Compact and efficient transformer-based model fine-tuned on general semantic similarity benchmarks; well-suited for low-latency applications.
	multi-qa-MiniLM-L6-cos-v1 (Thakur et al., 2021)	MiniLM variant fine-tuned specifically for multi-domain QA tasks using cosine similarity for improved dense retrieval accuracy.
	Msmarco-distilbert-base-v4 (Reimers& Gurevych, 2020)	DistilBERT-based model trained on the MS MARCO dataset for document and passage-level QA and retrieval tasks.
	nli-roberta-base-v2 (Reimers& Gurevych, 2019)	RoBERTa-based embedding model fine-tuned on natural language inference data, emphasizing sentence-level semantic alignment.
Our Embedding Models	HydroEmbed-OpenQA-MiniLM-DualLoss	Domain-specific Open-Ended QA model fine-tuned with CosineSimilarityLoss + MNRL to balance semantic alignment and discriminative power in free-form responses.
	HydroEmbed-FITB-MiniLM-DualLoss	Domain-specific Fill-in-the-Blank model fine-tuned with TripletLoss + CosineSimilarityLoss for precise cloze-style completions.
	HydroEmbed-MCQTF-MiniLM-MNRL	Domain-specific MCQ & True/False model fine-tuned using MNRL for semantic discrimination among closely related answer options.

For the FITB task, the model fine-tuned with both TripletLoss and CosineSimilarityLoss yielded an average cosine similarity of 0.9312, closely rivaling the top-performing ada-002 (0.9483) and surpassing all open-source baselines, including multi-qa-MiniLM-L6-cos-v1 (0.8048) and MiniLM-L6-v2 (0.8060).

On the Open-Ended task, which demands nuanced semantic understanding, the dual-loss (MNRL + CosineSimilarityLoss) fine-tuned model reached an average cosine similarity of 0.8053. This represents a substantial improvement over open-source baselines like MiniLM-L6-

v2 (0.7540) and nli-roberta-base-v2 (0.6506), narrowing the gap to high-performing proprietary models such as text-embedding-3-large (0.7750) and text-embedding-ada-002 (0.9242).

Table 3: Comparative Performance of Baseline and Fine-Tuned Embedding Models Across QA Formats in Hydrological Domain

	Model	**MCQ/TF Count**	**Accuracy**	**FITB Count**	**Avg. cos(θ)**	**Open-Ended Count**	**Avg. cos(θ)**
CLOSE	text-embedding-3-large	200	95.5%	100	0.8357	100	0.7750
	text-embedding-3-small	200	95.5%	100	0.8280	100	0.7595
	text-embedding-ada-002	200	95.0%	100	0.9483	100	0.9242
OURS	HydroEmbed-OpenQA-MiniLM-DualLoss	—	—	—	—	100	0.8053
	HydroEmbed-FITB-MiniLM-DualLoss	—	—	100	0.9312	—	—
	HydroEmbed-MCQTF-MiniLM-MNRL	200	93.5%	—	—	—	—
OPEN	all-MiniLM-L6-v2	200	93.0%	100	0.8060	100	0.7540
	msmarco-distilbert-base-v4	200	93.0%	100	0.7656	100	0.7005
	multi-qa-MiniLM-L6-cos-v1	200	94.5%	100	0.8048	100	0.7539
	nli-roberta-base-v2	200	93.0%	100	0.7656	100	0.6506

3.4. Discussion

The evaluation results demonstrate that the fine-tuned sentence embedding models yield significant improvements over general-purpose baselines, particularly in semantically complex tasks such as FITB and Open-Ended QA. These tasks require precise understanding of domain-specific language, contextual relationships, and lexical variability, capabilities that general-purpose embeddings often lack. For instance, the FITB model trained using both TripletLoss and CosineSimilarityLoss achieved an average cosine similarity of 0.9312, outperforming strong baselines such as all-MiniLM-L6-v2 and msmarco-distilbert-base-v4. Similarly, the Open-Ended model fine-tuned with a combination of CosineSimilarityLoss and MNRL achieved a cosine similarity of 0.8053, indicating stronger alignment with ground-truth responses than open-source alternatives.

These improvements highlight the critical role of loss function design in embedding model fine-tuning. Dual-loss configurations allowed the models to simultaneously optimize semantic closeness and discriminative separation, enabling robust generalization across paraphrased or structurally diverse responses. Particularly in Open-Ended QA, where response phrasing can vary significantly, the incorporation of contrastive signals was essential to prevent embedding collapse and preserve semantic granularity.

This design choice was guided by prior evidence from sentence-transformer research indicating that combining absolute-similarity and contrastive objectives enhances both semantic coherence and discriminative precision (Reimers & Gurevych, 2019; Sajja et al., 2025c). In Table 3, dual-loss configurations for FITB and Open-Ended QA yield higher alignment scores in semantically complex tasks, whereas the single-loss MNRL configuration performs optimally for structured formats such as MCQ and TF. These complementary patterns indirectly validate our rationale that the optimal loss design depends on task-specific linguistic and semantic demands. Because the study's primary aim was to evaluate domain-specific embedding adaptation rather than conduct a full optimization analysis, a dedicated ablation was considered beyond scope. Nevertheless, the observed performance patterns support the effectiveness and theoretical grounding of the adopted dual-loss strategies.

While fine-tuned models demonstrated strong task-specific gains, particularly in generative QA formats, performance in MCQ and TF tasks showed more modest improvements. With fewer answer options and clearer ground-truth targets, general-purpose embeddings already performed well. Nevertheless, the MCQ/TF model fine-tuned using MNRL reached 93.5% accuracy, approaching the performance of proprietary systems such as OpenAI's text-embedding-3-large, which reached 95.5%. These results affirm the value of fine-tuning even for structured QA formats, especially when contextual grounding and interpretability are important.

Importantly, these findings underscore the necessity of domain-specific embedding models in constructing robust RAG pipelines, QA systems, and scientific knowledge assistants. In domains like hydrology and environmental science, where texts are characterized by technical vocabulary, specialized syntax, and dense contextual dependencies, generic embeddings often fail to retrieve semantically relevant passages. Without effective semantic retrieval, even high-performing LLMs are constrained by poor context input leading to hallucinated or uninformative outputs. Thus, the quality of the embedding model becomes a foundational component of the RAG stack. While GPT-4o mini serves as a constant reader model in our RAG pipeline, future work will explore decoder-agnostic evaluation (e.g., context relevance metrics, zero-shot scoring) and human or multi-reference assessment to further isolate the contribution of the embedding models.

While our held-out evaluation set is instance-disjoint from training, we acknowledge that both are drawn from textbook sources. Two aspects mitigate overfitting risks in this setting: (i) the training signal is limited to QA pairs, whereas evaluation requires retrieval over chunked passages unseen during training, and (ii) models were trained with weight decay and warmup scheduling to curb memorization. Nonetheless, broader generalization should be assessed under stronger domain shifts. As next steps, we will conduct leave-one-textbook-out analyses and enable external-corpus evaluation by indexing article content for retrieval, thereby testing cross-source and cross-style robustness within the HydroLLM framework.

Moreover, as scientific and technical QA systems increasingly support use cases such as digital field assistants, real-time policy guidance, and adaptive learning environments, embedding models must be tuned not only for accuracy but for domain alignment and interpretability. The results of this study suggest that task- and domain-aligned fine-tuning strategies, particularly those leveraging contrastive learning, can significantly improve retrieval precision and downstream answer quality. However, further work is needed to improve robustness across document formats (e.g., research articles), develop adaptive chunking methods, and explore integration with external knowledge bases or ontologies to support more complete information grounding. In addition, future work will incorporate statistical significance testing (e.g., bootstrap resampling or paired comparisons) to more rigorously quantify performance differences between models.

3.4.1. Error and Confusion Analysis

To further understand the strengths and weaknesses of each fine-tuned model, we conducted a qualitative error analysis on a random subset of 50 examples per QA format. Errors were categorized by linguistic and retrieval characteristics. Across formats, we observed three dominant error types: (i) semantic overlap errors, where the model retrieved passages that were topically relevant but semantically adjacent to the ground-truth answer (e.g., retrieving “surface runoff” content for a question about “baseflow”); (ii) lexical ambiguity and synonym confusion, particularly in FITB and Open-Ended tasks where hydrological terms exhibit subtle contextual differences (e.g., “drainage basin” vs. “catchment area”); and (iii) context truncation, arising when relevant information spanned multiple chunks beyond the fixed-length retrieval window.

For True/False questions, a minor but consistent weakness involved negation handling (e.g., misinterpreting “not directly proportional”). Open-ended questions showed the highest semantic variance, reflecting the challenge of aligning model representations with descriptive explanations. Despite these limitations, most errors occurred in boundary cases involving overlapping domain terminology rather than fundamental comprehension gaps. This suggests that further improvements may be achieved through ontology-guided embedding refinement or adaptive chunking strategies in future work.

3.4.2. Toward HydroLLM: Domain-Specific Language Model for Hydrology

This study lays the groundwork for the broader vision of developing HydroLLM, a comprehensive domain-specific language model ecosystem for hydrology and environmental sciences. While the current work focuses on sentence-level embedding models optimized for retrieval and question answering, it serves as an essential step toward building full-scale generative and reasoning capabilities tailored to the unique linguistic, conceptual, and interdisciplinary demands of this domain.

The vision behind HydroLLM is to create a language model stack capable of understanding hydrological processes, environmental phenomena, and scientific discourse with the depth and accuracy needed for educational, operational, and policy-driven applications. This includes not only fine-tuned embeddings but also fully integrated large language models that can support scientific tutoring systems, environmental simulation interfaces, digital field assistants, and adaptive learning platforms.

Achieving this vision will require future work in several directions. These include expanding the training corpus to cover more diverse subfields (e.g., hydrogeochemistry, ecohydrology), integrating structured scientific knowledge bases and ontologies, developing document-aware and multimodal architectures, and evaluating performance on real-world decision-making tasks. Moreover, ensuring transparency, accessibility, and ethical deployment will be central to making HydroLLM a trustworthy tool for researchers, educators, and practitioners in the environmental sciences.

In addition to specialized embedding models for individual formats, a key future direction of HydroLLM is the development of unified or multi-task architectures capable of handling multiple QA formats within a single model. Such architectures would enable cross-format robustness, allowing the model to leverage shared semantic structures while adapting to task-specific requirements through conditional prompting or modular heads. This approach would help balance the trade-off between specialization and adaptability, advancing HydroLLM toward a more flexible and general-purpose domain-specific language model.

4. Conclusion

This study presents a comprehensive exploration of fine-tuned sentence embedding models specifically adapted for hydrology and environmental sciences. By leveraging the HydroLLM Benchmark dataset and applying tailored contrastive learning strategies, we demonstrate that adapting general-purpose embeddings such as all-MiniLM-L6-v2 to domain-specific contexts results in measurable gains in both answer accuracy and semantic similarity across a range of QA formats. These findings reinforce the hypothesis that domain-specific fine-tuning is essential for high-precision semantic retrieval and reasoning in specialized scientific fields.

The adoption of task-specific training objectives was a critical design decision. For MCQ and TF tasks, Multiple Negatives Ranking Loss enabled the model to effectively distinguish between closely related candidate options. For FITB tasks, combining Triplet Loss with Cosine Similarity Loss allowed the model to learn both semantic proximity and relative ranking between correct and incorrect completions. In the case of Open-Ended questions, where semantic nuance and answer variability are highest, the dual use of Cosine Similarity Loss and MNRL proved effective in capturing both absolute and contrastive relationships between input-output pairs. These design choices resulted in strong downstream performance, especially in FITB and Open-Ended tasks, where general-purpose models typically underperform.

The results also underscore the importance of embedding quality in end-to-end QA pipelines. In scenarios such as RAG, domain-specific embedding models serve as a foundation for locating relevant information before answer generation can occur. Without effective embedding alignment to the vocabulary and structure of domain-specific texts, such as those found in hydrology, LLMs may fail to retrieve or contextualize appropriate information, even when they have sufficient generative capabilities. In addition to accuracy, the HydroEmbed models are highly efficient for deployment: each contains only 22.7M parameters (~86 MB), requires ~0.10 GB of GPU memory during encoding, and achieves sub-6 ms single-query latency on an

NVIDIA RTX 3060. Because document embeddings are precomputed offline in our RAG setup, online inference involves only one query encoding and a fast nearest-neighbor lookup, making the models suitable for real-time or resource-limited environmental monitoring systems.

Beyond benchmark performance, these gains have direct implications for real-world hydrological applications. Improved semantic retrieval and QA alignment enable models to assist in tasks such as interpreting groundwater level projections under climate change, identifying sensitive variables in scenario analysis, synthesizing multi-model outputs, and supporting decision frameworks such as game-theoretic evaluations of groundwater exploitation. Domain-specialized embeddings can also enhance environmental monitoring tools by surfacing relevant scientific evidence, explaining spatial and temporal trends, and providing transparent, context-aware responses. Thus, the proposed models serve not only as technical improvements in retrieval accuracy but as foundational components for future decision-support systems, scientific assistants, and educational platforms in hydrology and environmental science.

Nevertheless, limitations remain. Open-Ended QA continues to be sensitive to the quality of retrieved context, and evaluation is constrained by the inability to retrieve or chunk article-derived content reliably. Rather than simply increasing the number of retrieved chunks (e.g., top-5), which often dilutes relevance with additional noise, we anticipate greater gains from more principled retrieval improvements. These include adaptive-k strategies that stop retrieval once similarity drops below a threshold, diversity-aware methods (e.g., MMR or submodular coverage) to reduce lexical redundancy, smarter chunking strategies that preserve sentence and section boundaries, and lightweight reranking to prioritize semantically faithful evidence. These retrieval refinements are especially important for open-ended tasks and represent a key direction for future work.

Future work will explore three principal directions. First, we aim to expand the training dataset by incorporating more QA pairs from additional textbooks and scientific publications, as well as real-world sources such as field reports, sensor-derived narratives, and policy or regulatory documents, alongside synthetic data augmentation techniques. Second, we plan to investigate the use of larger base models such as MPNet, GTR, and the latest open-weight LLMs for embedding generation, with the goal of improving semantic abstraction and generalization capacity. Finally, we will explore enabling multi-document reasoning and article-based evaluation by reformatting and indexing research article content to support reliable context retrieval. In addition to QA, these domain-specific embeddings can be extended to broader retrieval tasks such as temporal inference, document ranking, and evidence aggregation for forecasting or hybrid modeling pipelines, making HydroEmbed a foundational component for decision-support and scientific analysis in environmental systems. Additionally, we plan to explore multilingual and cross-lingual extensions to support global environmental data sources and international policy contexts.

Through this work, we contributed a suite of reusable, transparent, and domain-specialized embedding models optimized for semantic accuracy in hydrology and environmental science. These models lay the groundwork for future systems in scientific QA, intelligent tutoring, environmental information systems, and other applications requiring deep alignment with technical language and domain-specific reasoning.

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Availability of Data and Materials

The fine-tuned embedding models are released as open-source resources and can be accessed on Hugging Face at the following link: https://huggingface.co/HydroEmbed

Competing Interests

The authors declare that they have no competing interests.

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