Responses to Reviewer:

[Authors' response] We would like to sincerely thank the reviewer for his/her supporting and for taking the time to review our manuscript. Your good suggestions have increased our papers quality. thank you very much!

To Reviewer 1:

The paper presents a novel and well-structured inversion framework combining BPNN surrogate modeling with the AHA optimization algorithm for groundwater contamination source identification. The methodology is sound and the results are promising. The paper is generally well-written, but could benefit from some improvements in organization, clarity, and depth of discussion in certain sections.

General comments:

1. The introduction provides good background but could better highlight the novelty of the work compared to previous studies. What specific gaps does this study address that haven't been adequately covered before?

[Authors' response] We are very grateful to the reviewer for your valuable comments on the innovation of this study. To more clearly demonstrate the unique contributions of this study, we will further emphasize the research gaps and corresponding technological innovations in the introduction. Thank you again for your careful guidance and valuable suggestions!

2. For the surrogate modeling section, it would be helpful to provide more details about

the architecture of the BPNN (number of layers, nodes, etc.) and how these were determined.

[Authors' response] We appreciate the reviewers' attention to and suggestions regarding the architectural details of the BPNN proxy model. We will include detailed explanations of the relevant network structures in the revised manuscript. Specifically: The network structure of Case 1 BPNN is 19-30-45, and the network structure of Case 2 BPNN is 15-20-50. The number of neurons was empirically optimized using grid search and cross-validation to minimize RMSE and avoid overfitting. The sigmoid function is used as the activation function, and the Bayesian regularization algorithm is selected as the training algorithm. The learning rate is set to 0.01, and the maximum number of iterations is 1,000. Thank you again for your careful guidance and valuable suggestions!

3. The robustness analysis is good, but could be strengthened by showing how the errors distribute across different parameter types (e.g., are some parameters more sensitive to noise than others?).

[Authors' response] We thank the reviewer for this thoughtful suggestion. To enhance the robustness analysis, we conducted an additional evaluation of how the relative error varies among different types of inversion parameters under increasing noise levels (0.5%, 1%, and 2%).

Our findings reveal clear differences in sensitivity to noise among parameter categories:

Hydraulic conductivity (K values): These parameters showed low sensitivity to noise, with relative errors remaining below 3% in all scenarios for both PSC and ASC cases. Their errors increased gradually with noise but remained stable, indicating strong robustness. Boundary head values (H_1, H_2) (PSC case only): These parameters also exhibited excellent noise resistance, with relative errors consistently below 1% even at 2% noise level. Source release intensities (S values): This group showed the highest sensitivity to noise. At a 2% noise level, some source parameters (e.g., S_1T_1 in PSC, S_1T_3, S_1T_4, S_3T_2, S_3T_3, S_3T_5 in ASC) had relative errors exceeding 6%–10%, reflecting their higher inversion uncertainty under noisy conditions. This analysis has been summarized in the revised manuscript to better highlight parameter-specific sensitivities. These results underscore the need for targeted noise-reduction strategies (e.g., preprocessing) for more sensitive parameters in future work. Thank you again for your careful guidance and valuable suggestions!

4. The discussion of limitations is good but could be expanded. For example, how might the method perform with more complex, heterogeneous aquifers? What are the computational limits?

[Authors' response] We sincerely appreciate the reviewer's constructive feedback. In response, we have expanded the discussion to further elaborate on the limitations regarding aquifer complexity and computational feasibility.

First, with respect to aquifer complexity, the current study focuses on spatially inhomogeneous but isotropic aquifers under steady-state flow assumptions. However, in real-world hydrogeological systems, aquifers are often strongly heterogeneous and anisotropic, with nonlinear flow and transport dynamics. Applying the proposed inversion framework to such complex systems would introduce several challenges, including increased dimensionality of inversion variables, heightened parameter correlation and non-uniqueness, and difficulties in capturing highly irregular input–output relationships using surrogate models. These issues could compromise both the accuracy and stability of the inversion process. To address these challenges in future studies, techniques such as geostatistical priors, spatial regularization constraints, and multi-fidelity surrogate modeling could be incorporated to improve performance under realistic conditions.

Second, regarding computational limits, the integration of a surrogate model (BPNN) significantly improves computational efficiency by avoiding repeated calls to the numerical simulation model during optimization. In our current implementation, thousands of optimization iterations can be completed within a few minutes. However, as the complexity of the inversion problem increases (e.g., transitioning to 3D domains, transient scenarios, or reactive transport), the number of required samples and surrogate training time would increase substantially. The dimensionality of the decision variables also plays a critical role in determining the size of the training set needed to maintain surrogate accuracy. Additionally, while BPNN are relatively lightweight, deeper networks or ensemble-based surrogates may demand greater computational resources. Potential solutions to mitigate these issues include parallel computing, adaptive sampling, and hybrid surrogate strategies that balance accuracy and efficiency. Thank you again for your patient guidance and suggestions.

5. The practical implications section could be expanded. How would this method be implemented in real-world remediation projects?

[Authors' response] We thank the reviewer for the important question. In real-world groundwater contamination scenarios, the proposed surrogate-assisted inversion framework demonstrates effectiveness in identifying contamination sources, particularly when field data are limited, hydrogeological information is incomplete, and contamination source history is complex or unknown. The framework is typically implemented through a series of coordinated steps.

The process begins with an initial field investigation to collect spatiotemporal distribution data on contaminant concentrations from monitoring wells and obtain key information such as aquifer structure and boundary conditions. Although these data may be sparse and uncertain, they form the basis for inversion observations. Based on expert judgment and site-specific details, the study area is divided into subregions reflecting potential contaminant source locations, spatial variations in hydraulic conductivity, and uncertain boundary conditions. This partitioning establishes a framework for parameter inversion. Subsequently, a site-specific numerical groundwater flow and transport model (e.g., MODFLOW, MT3DMS) is developed to simulate contaminant migration. Through systematic sampling within a reasonable range, the model generates a set of training samples. These samples provide the data required to train a backpropagation neural network (BPNN) proxy model, which subsequently replaces the computationally intensive numerical simulation model to enable faster forward simulation. To identify the optimal parameter combination, the AHA is then applied to efficiently search the high-dimensional parameter space. This optimization process aims to find the optimal combination of parameters to minimize the difference between predicted and observed concentrations. The inversion results can reconstruct the spatiotemporal distribution of pollutant release, providing important evidence for guiding subsequent investigations, determining pollution responsibility, and formulating remediation plans. By effectively integrating observational data, numerical modeling, and intelligent optimization within a flexible and efficient framework, this method offers a practical solution for identifying pollution sources in complex and data-scarce groundwater systems. Thank you again for your patient guidance and suggestions!

6. Lines 231: While the proposed BPNN-AHA framework presents a robust approach, the authors may wish to consider and discuss alternative methodologies such as data assimilation techniques, which have shown promise in similar environmental modeling applications. For instance, data assimilation and cite paper such as Assimilation of sentinel-based leaf area index for modeling surface- ground water interactions in irrigation districts.

[Authors' response] We appreciate the reviewers' professional suggestions. We agree that data assimilation techniques, such as the ensemble Kalman filter or particle filter, have been widely applied in environmental modeling, particularly demonstrating good results in surface-groundwater coupling and hydrological forecasting. The literature cited by the reviewers demonstrates the excellent combined application of data assimilation methods. We will include a discussion of this issue in the revised manuscript and incorporate the literature recommended by the reviewers to supplement the progress of data assimilation techniques in environmental modeling. Thank you again for your patient guidance and suggestions!