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 2:

Luo et al. present an inversion framework that combines BPNN surrogate modeling with the AHA optimization algorithm for groundwater contamination source identification, and they comprehensively evaluate the performance of different surrogate models. The work is generally well written. However, several significant issues must be addressed to improve the clarity of the paper. The most critical concern lies in the structure of the Introduction. Although the authors provide an extensive literature review, the research gap and the novelty of this study in relation to previous work are not clearly emphasized. Secondly, the Discussion section lacks depth, which substantially weakens the novelty and the implications of this study. Finally, the language throughout the manuscript should be thoroughly revised and polished before publication.

[Authors' response] We appreciate the reviewer' positive evaluation of the methodological framework of this paper and their valuable suggestions. Regarding the main issues with the structure of the introduction, we plan to rewrite and supplement this section to more clearly articulate the research gaps and innovative points of this study compared to existing work. Additionally, we will expand the discussion section

to conduct a more in-depth analysis of the theoretical significance and practical applicability of the proposed method. Furthermore, we plan to conduct a comprehensive revision of the language throughout the paper, including improving clarity of expression, eliminating redundant content, and standardizing terminology and grammatical expressions to enhance overall readability. Thank you again for your careful guidance and valuable suggestions!

Specific comments:

1. Lines 127-135 The authors are recommended to reorganize the research objectives. The current unclear objectives obscure the novelty of the paper. This confusion is caused by an unclear summary of the research gap.

[Authors' response] We appreciate the reviewers' feedback regarding the unclear expression of research objectives and the lack of clarity in summarizing research gaps. In response, we plan to reorganize the corresponding sections of the manuscript to concisely articulate our research objectives, ensuring that the significant contributions of this study are highlighted. Thank you again for your careful guidance and valuable suggestions!

2. Line 151 MODFLOW and MT3DMS are not packages.

[Authors' response] Thank you to the reviewers for pointing out the inappropriate use of terminology. We confirm that MODFLOW and MT3DMS should be referred to as numerical models rather than "packages." We will revise the wording on line 151 in the

revision to ensure the professionalism and accuracy of the terminology. Thank you again for your careful guidance and valuable suggestions!

3. Line 305 Replace “inhomogeneous” by “Heterogeneous”.

[Authors’ response] We appreciate the reviewers' comments regarding the terminology used. We agree that in the field of hydrogeology, “heterogeneous” is a more accurate and commonly used term than “inhomogeneous.” We will correct the relevant expressions in the revised version. Thank you again for your careful guidance and valuable suggestions!

4. Lines 387-389 The authors are suggested to combine this sentence with the previous paragraph to create a clearer contrast, which would make the comparison more striking. Additionally, I am skeptical about the reported runtime for the 1000 iterations. Considering that the model in this study is at the field scale, consists of only a single model layer, and uses a rather coarse grid discretization, a runtime of 500 hours seems excessively long.

[Authors’ response] We appreciate the valuable suggestions provided by the reviewers. Regarding the structural suggestions, we will adjust the paragraph around lines 387–389 and merge the sentence into the previous paragraph to enhance the coherence of the preceding and following content, making the argumentation more logical and fluent. We also sincerely thank the reviewers for pointing out the inaccuracies in the runtime description. After re-verification, we confirm that the original text stating “500 hours”

was incorrect. In the current computational environment, a single simulation takes approximately 3 minutes to complete, and the total runtime for 1,000 optimization iterations is approximately 50 hours. We sincerely acknowledge this error and thank the reviewers for providing the opportunity to correct it. Thank you again for your patient guidance and suggestions.

5. Lines 420-424 This section reads more like a repetition of the Introduction. It is recommended that the authors first present their own findings in the Discussion before comparing them with other studies. Additionally, emphasizing the implications of this study would greatly enhance the value of the paper.

[Authors' response] We thank the reviewer for this valuable suggestion. We agree that the opening part of the Discussion section (lines 420–424) currently repeats background information already provided in the Introduction and does not effectively transition into our key findings. In the revision, we will restructure this section by starting with a focused summary of our main results before moving into comparisons with related studies. Additionally, we will enhance this part by more clearly articulating the broader implications of our findings, particularly regarding the practical applicability of the framework for real-world groundwater contamination scenarios. Thank you again for your patient guidance and suggestions!

6. Lines 438-440 Please specify the advantages more clearly.

[Authors' response] We appreciate the helpful suggestions provided by the reviewer.

We agree that the current statements in lines 438-440 do not clearly and specifically summarize the advantages of this method. In the revision, we will clearly identify the key advantages of this framework. Thank you again for your patient guidance and suggestions!

7. Lines 483 Including the limitations is good. The authors are suggested to include limitations in a separate section.

[Authors' response] We appreciate the reviewer's suggestion regarding the presentation of the study's limitations. While we have included some discussion of limitations in the current manuscript, we agree that presenting them in a standalone section will improve clarity and help readers better understand the scope and applicability of our method. Thank you again for your patient guidance and suggestions!

8. Lines 501 The authors are encouraged to include more quantitative findings rather than just qualitative notifications.

[Authors' response] We appreciate the reviewers' suggestion to add quantitative results to the conclusion section. We agree that introducing specific numerical indicators will help improve the expression of the conclusion and better reflect the core findings of this study. Therefore, we will supplement the main quantitative results in the revision, such as relative error, R^2 value, and performance comparison of different surrogate models, to more clearly summarize the accuracy and advantages of the proposed method. Thank you again for your patient guidance and suggestions!