Responses to Editor and Reviewer:

[Authors' response] First of all, we sincerely thank the editors and reviewers for their support and taking the time to review our manuscript. Your good suggestions have increased our papers quality. And also thank the editors to spend more time on our paper in the submitting process, thank you very much!

To Reviewer 2:

The authors have addressed most of my concerns. However, one aspect remains unclear, which largely limits the novelty of this study. Although the authors have compared some of the results with previous studies and added discussion in the revised manuscript (Lines 462–480), it is still not very clear from these discussions that this study makes substantial progress or introduces new ideas compared to earlier studies. The discussion mainly highlights similarities and consistencies with prior work.

[Authors' response] We sincerely thank the reviewer for the constructive comment. We fully agree that clearly highlighting the substantial progress and the unique contributions of this study is essential for emphasizing its novelty. In the revised manuscript, we have strengthened the discussion section.

Previous studies related to GCI employed a variety of methods to conduct either single or simultaneous inversion characterization of pollution sources and to identify hydrogeological parameters of the model. Li et al. (2022) identified the number, location, and release history of pollution sources, while Li et al. (2008) focused on determining the hydraulic conductivities of a study site. Bai et al. (2022) utilized

inversion techniques to simultaneously characterize pollution sources and identify the hydraulic conductivities within their simulation models. While some studies have applied inversion to the boundary conditions of the simulation model (Jiao et al., 2019), fewer studies have simultaneously characterized pollution sources and identified both hydrogeological parameters and boundary conditions of the model. Source information, model hydrogeological parameters, and boundary conditions are all critical components of groundwater contamination simulation models. Inaccuracies in any of these components can affect the overall results of inversion, making it essential to identify all components simultaneously. Therefore, in the PSC case of this study, the release history of the pollutant source, the hydraulic conductivity of the model, and the specific head boundary values were simultaneously identified. This simultaneous identification of multiple key parameters enhances the reliability and effectiveness of decision support systems.

One of the main methodological motivations of this study is the integration of the BPNN surrogate model with the AHA for GCI. This choice is grounded both in the inherent characteristics of GCI problems and in the complementary mechanisms of the two methods. GCI is a typical high-dimensional, nonlinear, and ill-posed inverse problem. The mapping from observed contaminant concentrations to source characteristics and hydrogeological parameters is often multimodal and nonconvex. In such cases, surrogate models such as BPNN can provide a fast and flexible approximation to computationally demanding groundwater simulations, but their use inevitably introduces approximation errors into the inversion objective function. These

errors may create local irregularities in the objective function landscape, which can mislead optimizers and cause premature convergence—particularly when the optimization algorithm lacks a mechanism to balance exploration and exploitation adaptively. AHA offers notable advantages in addressing these issues. Its bio-inspired mode-switching strategy alternates dynamically between diversified search and focused search. In the early stages of optimization, the broad and varied exploration capability helps to survey the global search space and reduces the risk of becoming trapped in spurious local optima caused by surrogate-induced noise. As the search proceeds, the algorithm adaptively shifts toward more intensive exploitation, concentrating computational effort on promising regions and thereby accelerating convergence. This dynamic adjustment is particularly important in GCI problems, where the optimal parameter region is often narrow and embedded within a complex and noisy search space. In addition, AHA's adaptive update mechanism adjusts search trajectories in response to population feedback, effectively mitigating the influence of local fluctuations in the surrogate-predicted objective function on the optimization process. This robustness to noisy or irregular fitness landscapes complements the BPNN's ability to generalize across diverse contamination scenarios. It is worth emphasizing that this integration is not a simple "algorithm replacement," but a targeted design choice based on the structural characteristics of the problem: BPNN provides broad adaptability to varying hydrogeological conditions, while AHA contributes resilience and fine-tuning capability when the optimization landscape is distorted by surrogate approximation errors. This synergy allows the proposed framework to maintain both

high accuracy and strong robustness under different contamination scenarios and noise levels. More importantly, the underlying design principle—matching the characteristics of the surrogate model with the search dynamics of the optimization algorithm—has broader applicability to other environmental inversion problems. The modified content is highlighted in red. Please refer to lines 501-518 and lines 542-576 for details. Thank you again for your careful guidance and valuable suggestions!

Minor comments:

Lines 141-142 boundary conditions are not parameters. In addition, the innovations should be discussed in the context of other studies. Simply listing them in the introduction is not appropriate.

[Authors' response] We sincerely thank the reviewer for the constructive comment. We fully acknowledge that boundary conditions are not parameters, as this part of the original text has been revised. Additionally, in the discussion section, we further elaborate on the novelty of this study by contextualizing it within the background of other research. The modified content is highlighted in red. Please refer to lines 140-142, 501-518, and 542-576 for details. Thank you again for your careful guidance and valuable suggestions!

Lines 161-163 Here should cite the software developer, no?

[Authors' response] We appreciate the reviewer's valuable suggestion. We have cited the relevant software developers in the article. The additional content is highlighted in

red. Please refer to lines 160-161, 674-675, and 821-822 for details. Thank you again for your careful guidance and valuable suggestions!

Line 585 Aquifer system is more accurate.

[Authors' response] We appreciate the reviewer's valuable suggestion. We have changed the term "groundwater system" in the article to "aquifer system." The modified content is highlighted in red. Please refer to line 585 for detail. Thank you again for your careful guidance and valuable suggestions!

Remarks from the preceding review file validation:

Please note that your reference list has not been compiled according to our standards. Please consider adjusting your reference list with the next revision of your manuscript. The manuscript preparation guidelines can be seen at: https://www.hydrology-and-earth-system-sciences.net/for_authors/manuscript_preparation.html.

[Authors' response] Thank you very much for your suggestion. We have formatted the references throughout the manuscript according to the preparation guidelines. The modified content is highlighted in red. Please refer to lines 656-822 for details. Thank you again for your careful guidance and valuable suggestions!

1. A "Short summary" system section contains scientific abbreviations. Please be aware that if you included scientific abbreviations (excluding chemical elements) without providing their full written explanations, you must write out them in full in your next

file upload request. However, do not forget that there is a limit to characters (not words!) for “Short summary”: it must be < 500 characters.

[Authors’ response] We have fully expanded the abbreviation “BP neural network” in the “Short Summary” to “back-propagation neural network.” The total number of characters (including spaces) is 317, which is less than 500 characters. Thank you again for your careful guidance and valuable suggestions!

2. Please ensure that the colour schemes used in your maps and charts allow readers with colour vision deficiencies to correctly interpret your findings. Please check your figures using the Coblis – Color Blindness Simulator (https://www.color-blindness.com/coblis-color-blindness-simulator/) and revise the colour schemes accordingly with the next file upload request.

[Authors’ response] Thank you very much for your suggestion. We have used Coblis—Color Blindness Simulator—to review the images in this article, ensuring that the color schemes employed in the figures enable readers with color vision deficiencies to accurately interpret our findings. Thank you again for your careful guidance and valuable suggestions!

3. Regarding the section "Author contributions", we kindly ask you to use rather initials of the authors instead of full names in this section with the next revision.

[Authors’ response] Thank you very much for your suggestion. We have used the author's initials instead of their full names. The modified content is highlighted in red.

Please refer to lines 641-644 for details. Thank you again for your careful guidance and valuable suggestions!

4. Please add the figure captions directly beneath the respective figures.

[Authors' response] Thank you very much for your suggestion. We have added graphic titles directly below the corresponding figures. The modified content is highlighted in red. Please refer to lines 845-846, 848, 850, 852-853, 855, 857-858, 860-862, 865-866, and 868-869 for details. Thank you again for your careful guidance and valuable suggestions!

Thank you so much for your carefully review and good suggestions that make our paper quality improve. Best wishes for you and your whole family members!

Best wishes for you!

Sincerely

Chengming Luo, Xihua Wang, Y. Jun Xu, Qinya Lv, Xuming Ji, Boyang Mao, Shunqing Jia, Zejun Liu, Yanxin Rong, Yan Dai

August 28th 2025