Response to comments from Anonymous Referee #1

Overview of Anonymous Referee #1:

This paper, based on real basin study area, systematically analyzes the scale effects of solute transport and dispersion in heterogeneous aquifers using a hierarchical sedimentary framework and numerical simulation. Overall, the manuscript has a good topic selection and relatively advanced research methods, aligning with research frontiers in non-Fick solute transport in heterogeneous aquifers. Through detailed results presentation and comprehensive discussion, it provides practical guidance for large-scale modeling and groundwater management in data-limited regions. However, there is still some space for improvement in areas such as writing format, methodological hypotheses, quantification of results, and the applicability of the research.

Reply: We sincerely thank the reviewer for the constructive and insightful comments, which helped us improve the manuscript in terms of clarity, methodological transparency, quantification of key findings, and applicability. In the revised manuscript we will address each of his/her observations/suggestions.

Specific comments:

（1）In the Abstract and Discussion sections, authors mentioned "…prolonged pre-asymptotic phase, far exceeding that observed at classical sites such as Borden.", it is suggested that quantitative metrics can be provided here to make the difference in solute transport characteristics between sites and basins more intuitive. Furthermore, the authors mentioned "mechanistic and transferable framework" and "practical guidance" at the end of the Introduction section, but these are broad descriptions. A more accurate and intuitive expression would be better, such as which observable parameters are most important for predictable diffusion indices.

Reply: Thank you for this comment. We have revised the text of the **Abstract** and **Discussion** sections, added some quantitative metrics and provide more specific expressions. Below are the specific modifications in the tracking version manuscript.

The red content is the modified information, and the black content represents the original text (the same applies below).

In the **Abstract** section: The results reveal that the geometry and connectivity of dominant lithofacies at macroform scales control macro-dispersionmacrodispersivity, while finer-scale heterogeneity has only a secondary influence on plume evolution. Furthermore, the evolution of macro-dispersionmacrodispersivity is characterized by a prolonged pre-asymptotic phase, far exceedingapproaching a quasi-steady state after around 5000 days, with an asymptotic stability value of 170m. This timescale is nearly 10 times longer than that observedinferred from the Boden site, where macrodispersivity approaches the asymptote after approximately 400 days, stabilizing at classical sites such as Borden, indicatingaround 0.4m.

In the **Discussion** section**:** A central finding is the scale-dependent nature of plume stabilization. Over a 10000 days simulation period, dispersivity values$\alpha_{eff}(t)$ initially increased slowly and then stabilized. This indicates that after sufficient time, the plume's large-scale transport behavior begins to stabilize, reflecting a condition where the plume has sampled a representative portion of the large-scale heterogeneity. However,, but this stabilization occurs over an extremelya relatively prolonged period (around 5000 days) , highlightingindicating that plume evolution remains in a pre-asymptotic, or (quasi-ergodic,) state for thousands of days at the basin scale. By contrast, this differs significantly from findingsThis behaviour contrasts with site-scale results at the Borden site (Ren et al., 2022), where dispersivity$\alpha_{eff}(t)$ was shown to reach an asymptotic value much more rapidly (after 400 days), plausibly facilitated by higher mean groundwater velocities. In the present basin-scale system, the solute explores only a small fraction of the heterogeneous flow field over a considerable period of time, the effective transport response is “buffered” by the domain immensity. Source size exerts a qualitatively consistent effect across scales: expanding the source promotes broader early-time sampling of heterogeneity and thereby reduces inter-realization variability, yielding narrower uncertainty during transport process. By contrast, the uncertainty band for $\alpha(t)$ tends to stabilize or even decrease later at the basin scale, again reflecting domain scale averaging that mutes source geometry effects far downstream. In the site-scale tracer experiments (e.g., MADE, Borden), meter-scale *K* variability may lead to apparent velocities differ by orders of magnitude between observation points, and strongly connected preferential pathways commonly yield pronounced early arrivals and heavy-tailed breakthrough curves (Zheng et al., 2011; Bianchi and Pedretti, 2017), thereby increasing predictive uncertainty in plume evolution and arrival-time statistics. Simulations at the Borden site well demonstrate that the increased proportion of more permeable lithofacies significantly amplifies solute dispersion and output uncertainty. Basin-scale models, however, exhibit a weaker response, consistent with the buffering effect of long travel distance and multiple overlapping pathways.

（2）The last part of the Introduction section is the structure of the paper. It is suggested that word "part" can be changed to "section", and that the title of the Section 2 can be changed to "methods". Section 2.2.1 should be renamed to "Sedimentary heterogeneity parameters" or "Sediment heterogeneity parameters."

Reply: We agree and have revised the expression accordingly. We have replaced "part" with "section" in the Introduction section, and have renamed Section 2 to "Methods," and revised Section 2.2.1 to "Sediments heterogeneity parameters". Below are the specific modifications in the tracking version manuscript.

Revised information is in Line 103-107 in the tracking version manuscript: The paper is organized as follows: ~~Part~~Section 2 introduces the geographic background of the study area, borehole data, and sedimentary architecture analysis methods; ~~Part~~Section 3 describes the construction of the ~~multi-scale~~multiscale heterogeneous structural model and the simulation process of solute transport; ~~Part~~Section 4 shows the simulation results and conducts uncertainty analysis to explore the influence of sedimentary architecture and permeability parameters on solute dispersion; ~~Part~~Section 5 summarizes the main conclusions and ~~puts forward the~~outlines future research~~.~~ directions.

（3）In the text, background information and existing research should be described using the present or past tense; the Methods section of the paper should use the past tense or passive voice; the Results/Discussion section should use the present tense. Please make the corresponding modifications throughout the paper.

Reply: We have now systematically revised verb tense usage throughout the manuscript.

（4）57 boreholes were used to construct 20 km × 22 km × 50 m models in this study. While this is a common practice in basin scale modeling, its representativeness still needs to be effectively evaluated since this research focuses on the heterogeneity of the aquifer. It is recommended that the authors supplement the relevant content in the manuscript.

Reply: Thank you for raising the important issue of data representativeness. In fact, within a 20 km × 22 km area, this study used not only 57 boreholes but also 8 cross-sections as constraints to represent the potential heterogeneity of the aquifer. The primary objective of this study is not to reproduce a specific site plume deterministically, but to quantify how hierarchical sedimentary architecture and associated parameter uncertainties govern basin-scale dispersion under field-representative flow conditions. Consistent with common practice in regional/basin-scale hydrogeological modeling, we therefore treat the borehole data as hard constraints and rely on a hierarchical, transition-probability/Markov-chain–based geostatistical framework to stochastically populate the inter-borehole space and to explicitly quantify geological uncertainty through ensembles of conditional realizations. To more clearly address these considerations, we have added a new paragraph in the end of the Section 2.2.1.

Revised information is in Line 175-183 in the tracking version manuscript: In this study, the 57 boreholes provide hard conditioning data for facies occurrence and aquifer thickness, whereas the eight cross-sections supply additional structural constraints on lateral continuity and stratigraphic organization along and across the principal directions. This study is not aim to deterministically reproduce specific in-situ plumes, but rather quantifies how hierarchical sedimentary architecture and associated parameter uncertainties govern basin-scale dispersion under field-representative flow conditions. The resulting heterogeneous model was intended to be statistically representative, while local connectivity in data-poor areas was treated as uncertain and quantified through a set of conditionally realizations. Although boreholes and corresponding cross-sections are more densely packed in the central and western parts of the study area and relatively sparse in the eastern area, this is sufficient to serve the objectives of this study.

（5）A constant porosity of 0.35 is not sufficiently for facies ranging from gravel to clay, but this simplification is acceptable if the research objective is solely to resolve the control of the K-field and architecture on dispersions. It is recommended that the assumptions for this parameter be explicitly stated in Section 2.4.3, and that any potential biases introduced by these assumptions be briefly discussed in the discussion section. Similarly, setting D_{ij}=0 implies that macrodispersion is only caused by non-uniform velocity fields. This is reasonable for studying pre-asymptotic behavior of structural controls, but it might underestimate dispersion compared to real systems. It is recommended to add discussion of this aspect in the parameter settings and Discussion section.

Reply: Thank you for this comment. We have explicitly stated in Section 2.4.3 that the simplification of setting a constant porosity and neglecting the effects of local-scale dispersion and molecular diffusion is reasonable to identify the structural and *K*-field controls on macrodispersion. Setting $D_{ij} = 0$ implies that solute dispersion arises solely from non-uniform velocity fields (macrodispersion driven by heterogeneity/architecture), which is appropriate for diagnosing pre-asymptotic structural controls but could underestimate total dispersion relative to real aquifers where local dispersivity and molecular diffusion contribute. The limitations and applicability boundaries have also been discussed in both the Section 2.4 and the Discussion Section.

Revised information is in Line 261-267 in the tracking version manuscript: In this study, Θ ~~is~~was assumed to be stably isotropic and ~~takes~~was set to the value of 0.35. ~~The~~Although setting a constant porosity may lead to deviations in the time required to reach a certain stage and the absolute value of the dispersion index plotted on the time axis, this study, however, emphasized the influence of aquifer structure and *K*-statistics under consistent settings, where the spatial heterogeneity and connectivity of the corresponding velocity field were not significantly determined by subtle spatial variations in porosity. Another advantage of this choice is to avoid introducing other poorly constrained parameter fields into the model. For the same reason, the influence of local scale dispersion and molecular diffusion coefficient ~~were~~was not considered in this study, and therefore the corresponding dispersion and diffusion coefficients were taken as zero.

Revised information is in Line 504-508 in the tracking version manuscript: It must be acknowledged that neglecting porosity variations and molecular diffusion processes in this study may lead to an underestimation of early plume smoothing and lateral mixing, potentially delaying a significant convergence to Fick behaviour. However, at the basin scale and in the long-distance travel considered in this paper, structure-controlled velocity variations are expected to dominate the dispersion index; therefore, the main conclusions regarding relative lithofacies proportions and connectivity remain unchanged.

（6）The existing Uncertainty analysis section is a "scenario analysis" What is the basis for setting up the comparison groups for volume proportion and conductivity? In other words, is this reasonable in terms of geological conditions? Please provide further explanation or emphasize the application scenario of this setting to enhance the guiding significance of the conclusions.

Reply: Thank you for this comment. At the beginning of Section 3.2, we clarify that the uncertainty analysis is implemented as an scenario analysis. The scenario design was motivated by a published global sensitivity analysis indicating that facies volume proportions and in-facies mean hydraulic conductivity exert first-order influence on non-reactive solute dispersion across regional to basin scales. From a geological perspective, in fluvial–alluvial systems the relative abundance of channel-belt coarse deposits (e.g., gravel/sand bodies) versus floodplain fine deposits can vary substantially in planar terms, reflecting differences in depositional energy, channel migration/avulsion style, floodplain development, and base-level conditions. We therefore use proportional end members to represent plausible depositional settings. Specifically, Group A (near-equal proportions) represents a more mixed and interbedded architecture consistent with frequent channel migration and facies switching, whereas Group B (fine-dominated mixtures) represents a low-energy and/or distal floodplain setting where fine deposits are more prevalent and coarse bodies are more isolated. The mean-*K* perturbation scenarios keep the architecture fixed and any changes in dispersion can be attributed to altered inter-facies conductivity contrast and the resulting redistribution of flow among facies (K×3 corresponds to a medium to high level of hydraulic-property uncertainty). As is well known, hydraulic conductivity varies widely and is subject to considerable estimation and upscaling uncertainty at field scales. In summary, the chosen facies-proportion and mean-*K* groups represent plausible depositional/parameter-uncertainty end members for fluvial–alluvial plains and are intended to provide decision-relevant bounding behavior rather than posterior probabilistic estimates. To enhance the practical application guidance value of this study, we added a description of parameter value considerations in the Section 3.2.1 and Section 3.2.2, and provided the corresponding environmental scenarios.

Revised information is in Line 367-373 in the tracking version manuscript: From a sedimentological perspective, in fluvial–alluvial systems the areal proportion of coarse deposits (e.g., gravel/sand bodies produced in paleochannel zones) versus floodplain fine deposits can vary substantially at the basin scale, reflecting the coupled effects of stream power and sediment supply, channel migration, floodplain aggradation and development (Bridge, 2009). Accordingly, Group A (near-equal proportions) represents a more mixed and interbedded architecture consistent with frequent channel migration and facies switching, whereas Group B (fine-dominated mixtures) represents a low-energy and/or distal floodplain setting where fine deposits are more prevalent and coarse bodies are more isolated.

Revised information is in Line 415-423 in the tracking version manuscript: As is well known, *K* varies widely and is subject to considerable estimation and upscaling uncertainty at field scales. To isolate the role of individual lithofacies, three model groups were designed in which only the mean *K* of a single lithofacies was increased threefold, while the other two remained unchanged. The choice to expand by three times also takes into account the uncertainty of *K* at a medium to high level. In Group 1, the mean *K* of GCS was raised to 138.06 m/d, with MFS and SC fixed at 10.34 m/d and 0.12 m/d, respectively. In Group 2, the mean *K* of MFS was increased to 31.02 m/d and in Group 3, the mean *K* of SC was increased to 0.36 m/d. In all cases, the variance of *K* was preserved, and the underlying heterogeneous sedimentary architecture remained unchanged. Thus, all solute transport simulations were carried out within the same structural framework.Thus, any changes in dispersion can be attributed to altered inter-facies *K* contrast and the resulting redistribution of flow among facies.

（7）In the Results section, please focus on "presentation + brief explanation". Lengthy discussions about cross-scale or literature comparison can be systematically elaborated in the Discussion section to avoid repetition and redundancy of the text.

Reply: Thank you for this comment. We have optimized the description in the Results Section and focused on key outputs and concise explanations. Other extended cross-scale interpretations and literature comparisons have been moved to the Discussion Section.

（8）There are several grammatical issues in the text. For example, line 93, "less than < 1‰" should be modified to "< 1‰"; Line 175，"Scale-II" is recommended to be consistently referred to as "Scale II"; line 320，"…dispersivity shows a power…" is recommended to modified as "dispersivity exhibits a power-law increase with time.". Therefore, it is recommended that the authors carefully revise and polish the English writing throughout the manuscript.

Reply: Thank you for this comment. We have carefully revised and polish the English writing throughout the manuscript to solve such mistakes.

（9）In Figure 3, it is recommended to also mark key information such as the location of the Nen River and its upstream and downstream relationships.

Reply: We agree and have updated Figure 3.

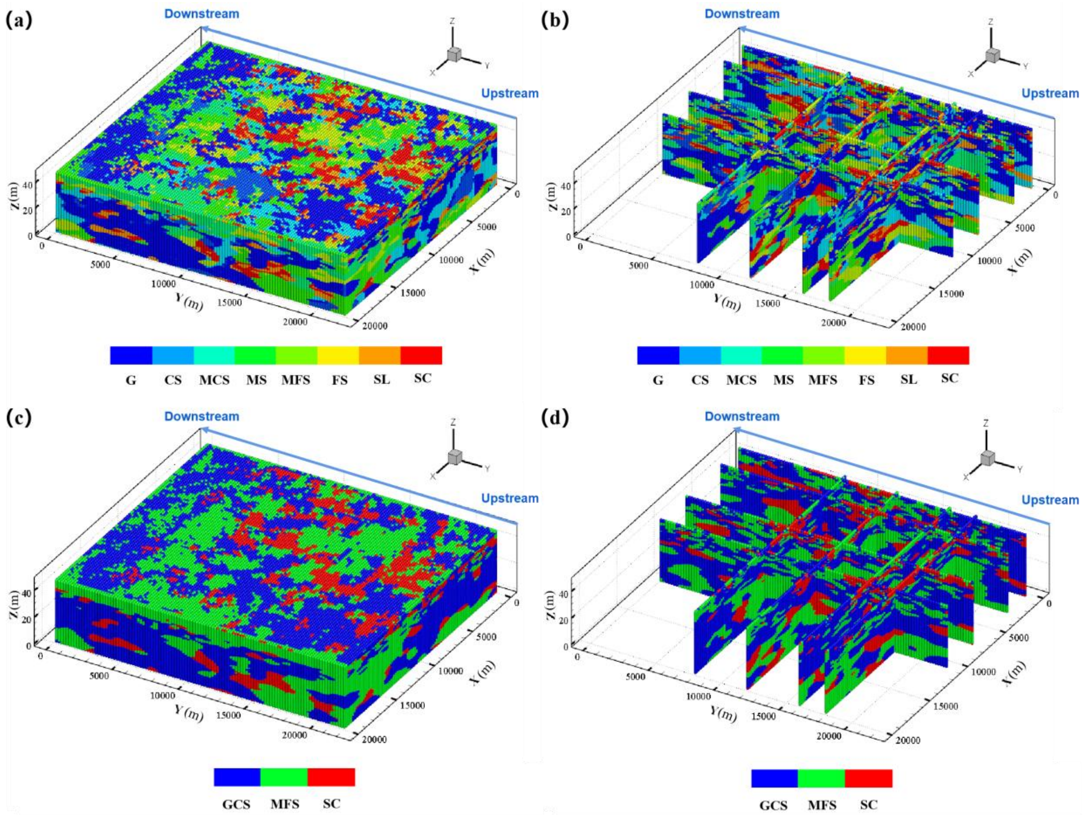

Figure 3. An example of multiscale model: (a) 3-D facies, (b) 2-D sections; and Scale II model: (c) 3-D facies, (d) 2-D sections. Section lines at *x* = 600m, 3000m, 7600m, 11000 m and *y* = 8000m, 12000m, 16000m, 18000m

（10）In Figure 2, it is suggested that "phreatic water aquifer" in the title should be changed to "phreatic aquifer" directly.

Reply: Thank you for this comment. We have modified the title as "**Schematic diagram of lithofacies composition of the layered structural model of Qiqihar phreatic ~~water~~ aquifer**".

（11）Regarding flow field calibration (in Figure 5), it is currently stated that "The simulated water levels show good agreement... closely following the 1:1 line.". although the trend looks good on the graph, but specific values such as RMSE, NRMSE, and R^2 are missing.

Reply: Thank you for this comment. Quantitative metrics are indeed necessary. We will add REMS to support the statement of good agreement.

Revised information is in Line 296-298 in the tracking version manuscript: The simulated water levels show good agreement with the observed values, closely following the 1:1 line~~, which proves~~. This visual consistency is supported by a relatively small error (RMSE = 0.507m), indicating that the water flow model ~~constructed in this study reliably captures~~reproduced the groundwater dynamics of the study area.